

Electronic Supplementary Information
for
**Chiral *N*-Triflylphosphoramidate-Catalyzed
Asymmetric Hydroamination of Unactivated Alkenes:
A Hetero-Ene Reaction Mechanism**

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1. Additional computational details

1.1 Model computational study

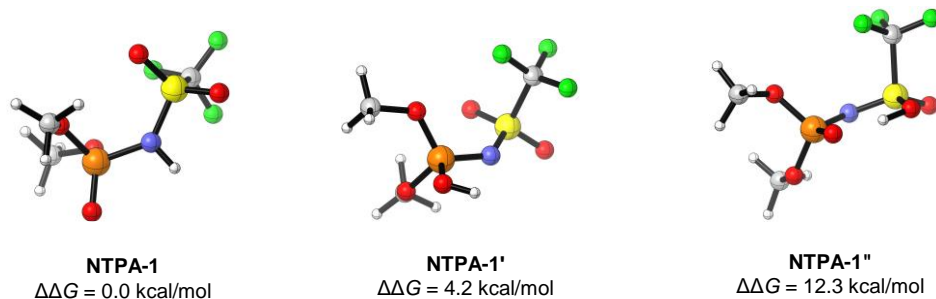


Fig. S1 Computed relative free energies of model *N*-triflylphosphoramidate **NTPA-1** and its tautomers at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Free energies are referred to that of **NTPA-1**.

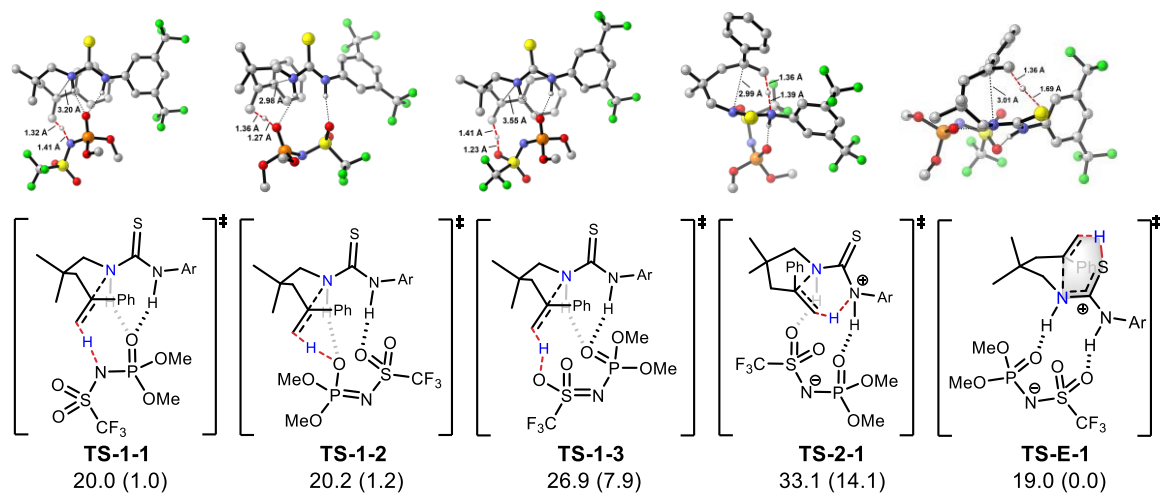


Fig. S2 Computed activation energies (ΔG^\ddagger in kcal/mol) of different pathways and 3D structures of corresponding transition states for the model reaction at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies ($\Delta\Delta G^\ddagger$ in kcal/mol) are given in parenthesis and are referred to that of **TS-E-1**.

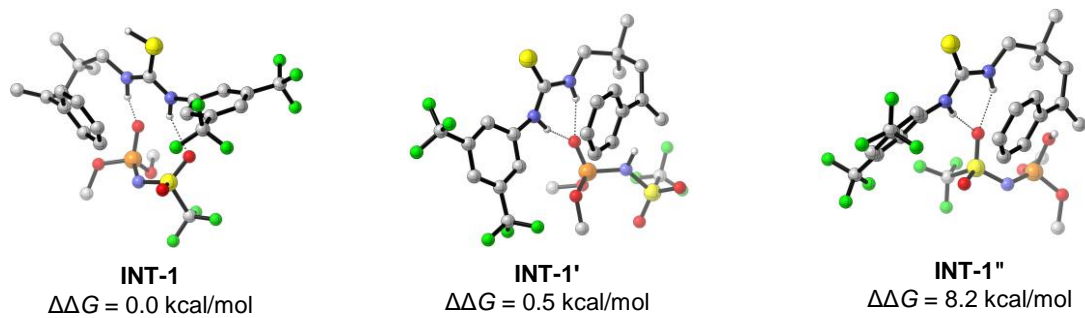


Fig. S3 Computed relative free energies of precomplexes along different reactions pathways for the model reaction at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to that of **INT-1**.

1.2 The reaction of **AT-1** catalyzed by **NTPA-2R**

1.2.1 Comparison of the electronic and free energy differences of enantio-determining transition states calculated with different methods

For comparison with the B3LYP energies, geometry optimizations were also performed using the B3LYP-D3(BJ), ω B97X-D, and M06-2X functionals together with the 6-31G(d) basis set for the transition states (**TS-EF-1S** & **TS-EF-1R**) along the heteroene reaction of **AT-1** catalyzed by **NTPA-2R**. Single-point energy calculations were calculated using the M06-2X functional together with the 6-311+G(d,p) basis set. The SMD model was used to account for solvent effects. Computations with B3LYP and ω B97X-D were found to provide close agreement with the experimentally observed stereoselectivity. In addition, single-point energies were also evaluated within the SMD model using the ω B97X-D and B3LYP-D3(BJ) functionals, which provided comparable enantioselectivities.

Table S1. Electronic and free energy differences of enantio-determining transition states calculated with different methods

Entry	Method	$\Delta\Delta E_{(R-S)}$	$\Delta\Delta G_{(R-S)}$
1	SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d)	1.2	2.0
2	SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP-D3(BJ)/6-31G(d)	3.9	3.5
3	SMD(DCM)-M06-2X/6-311+G(d,p)// ω B97X-D/6-31G(d)	3.2	1.8
4	SMD(DCM)-M06-2X/6-311+G(d,p)//M06-2X/6-31G(d)	1.4	1.0
5	SMD(DCM)- ω B97X-D/6-311+G(d,p)//B3LYP/6-31G(d)	1.1	1.9
6	SMD(DCM)-B3LYP-D3(BJ)/6-311+G(d,p)//B3LYP/6-31G(d)	1.8	2.6
Experimental result		(S)- 1 , 94% ee	

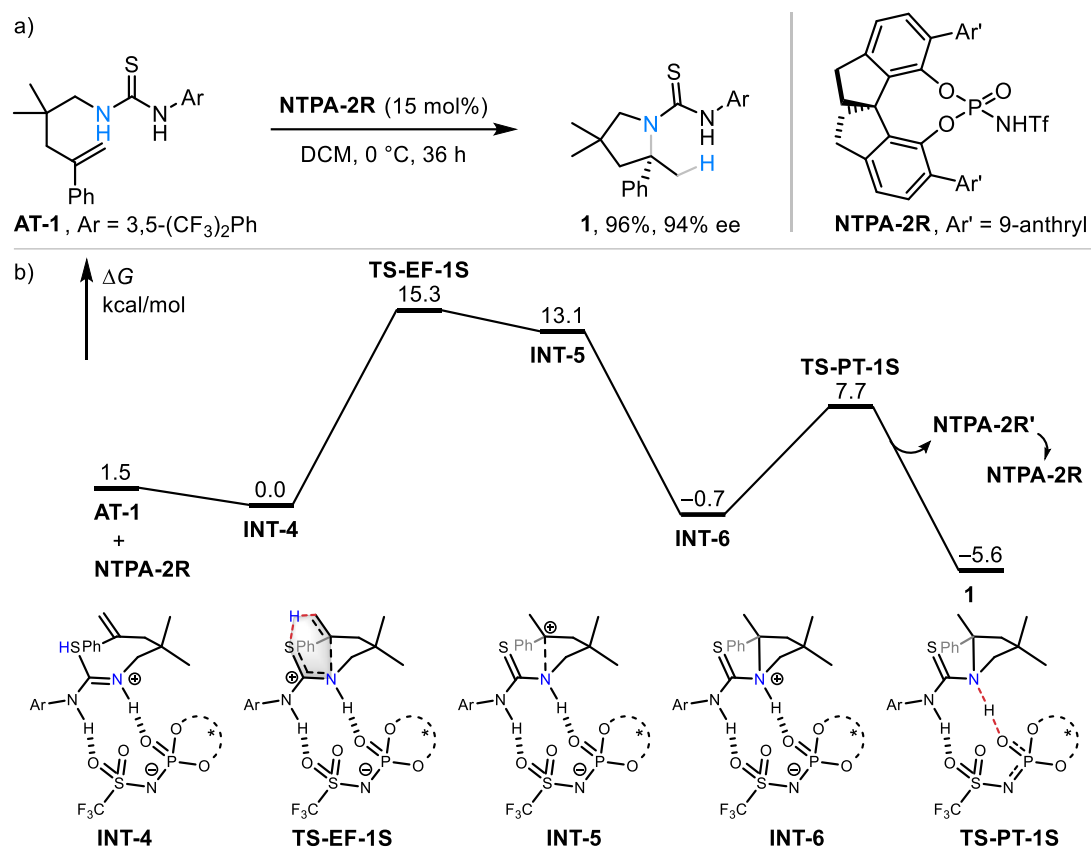


Fig. S4 (a) Experimental results of the hydroamination reaction of **AT-1** catalyzed by **NTPA-2R**. (b) Free energy profile of the most favorable hetero-ene reaction pathway.

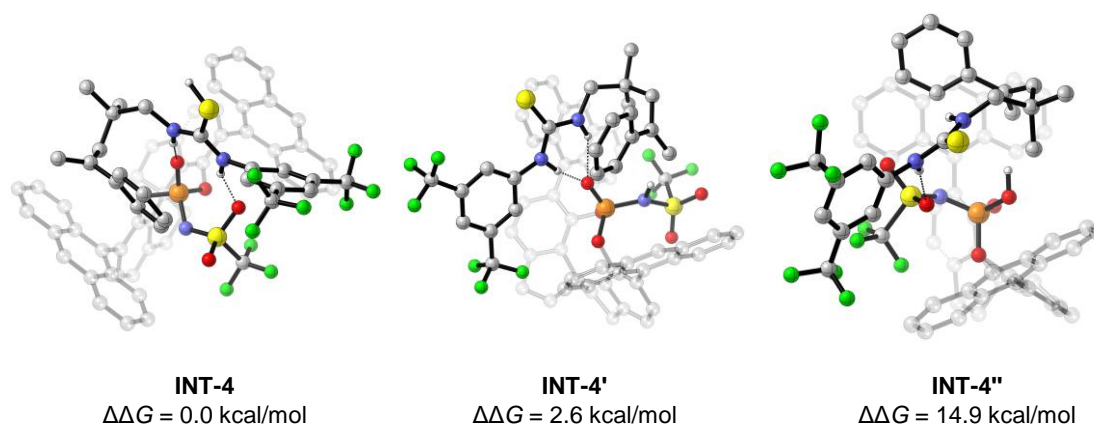
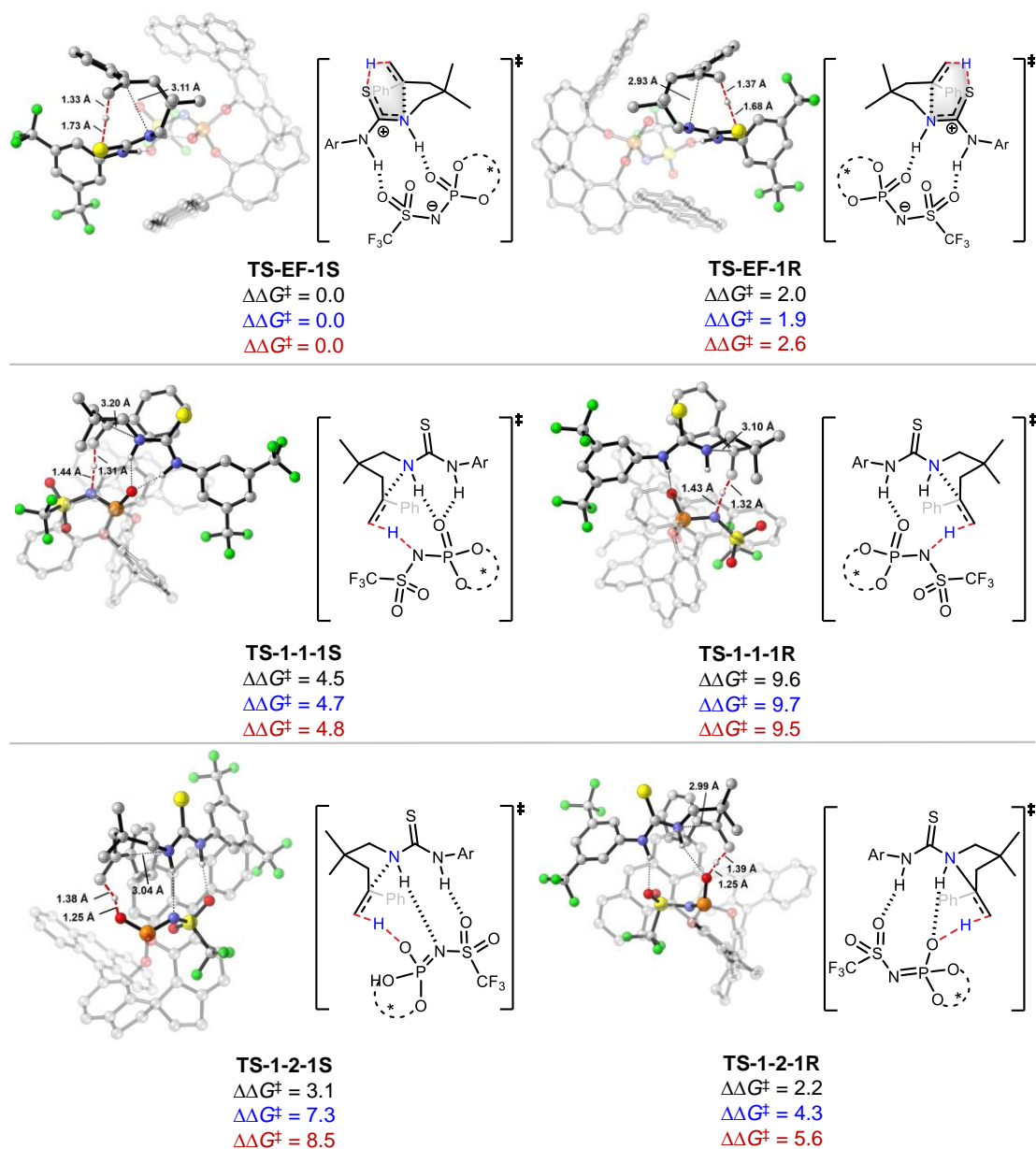


Fig. S5 Computed relative free energies of precomplexes along different reactions pathways for the reaction of **AT-1** catalyzed by **NTPA-2R** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to **INT-4**.



SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d)
SMD(DCM)- ω B97X-D/6-311+G(d,p)//B3LYP/6-31G(d)
SMD(DCM)-B3LYP-D3(BJ)/6-311+G(d,p)//B3LYP/6-31G(d)

Fig. S6 Computed favorable transition states of the reaction of **AT-1** catalyzed by **NTPA-2R** with three methods. Relative free energies are referred to **TS-EF-1S**.

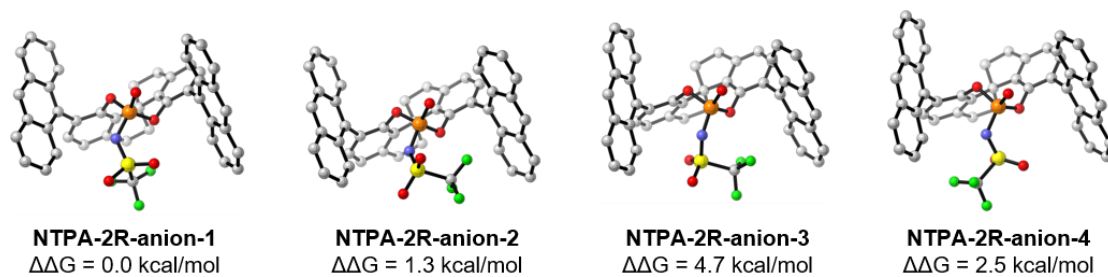


Fig. S7 Computed relative free energies of the *N*-triflylphosphoramidate anion at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to **NTPA-2R-anion-1**.

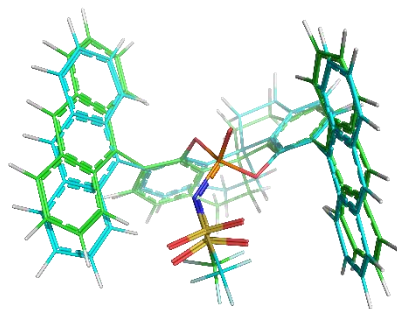


Fig. S8 Superimposition of the catalyst fragment in **TS-EF-1S** with the corresponding fully relaxed free structure **NTPA-2R-anion-1**. Carbons in **NTPA-2R-anion-1** are drawn in green while that in **TS-EF-1S** blue.

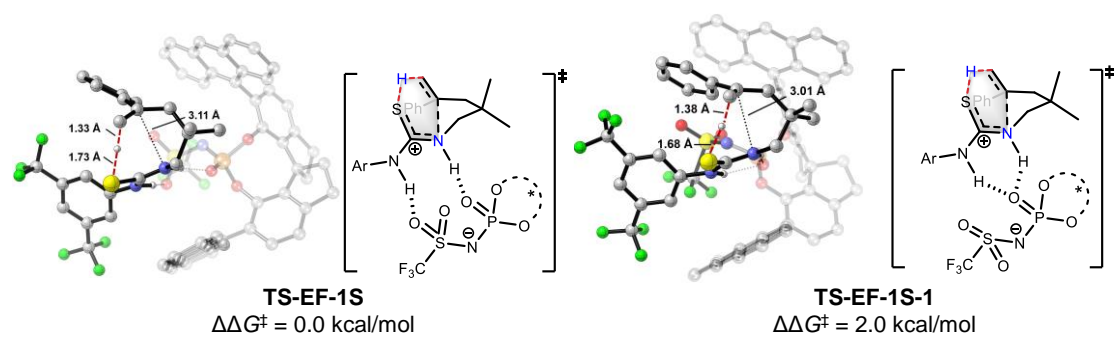


Fig. S9 The Importance of the triflyl moiety in forming hydrogen bonding for lowering the reaction barrier.

1.3 The reaction of **AT-2** catalyzed by **NTPA-2R**

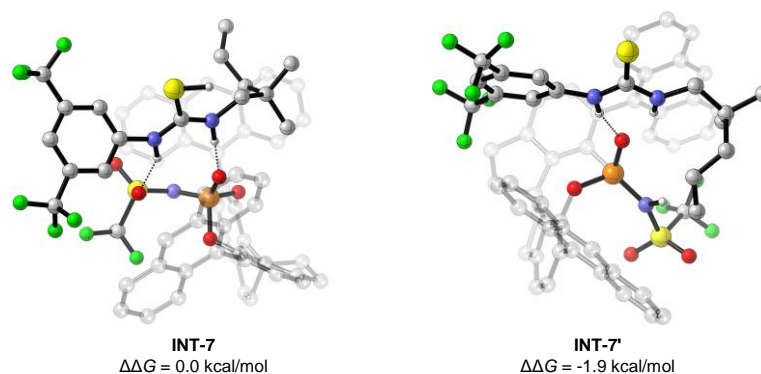
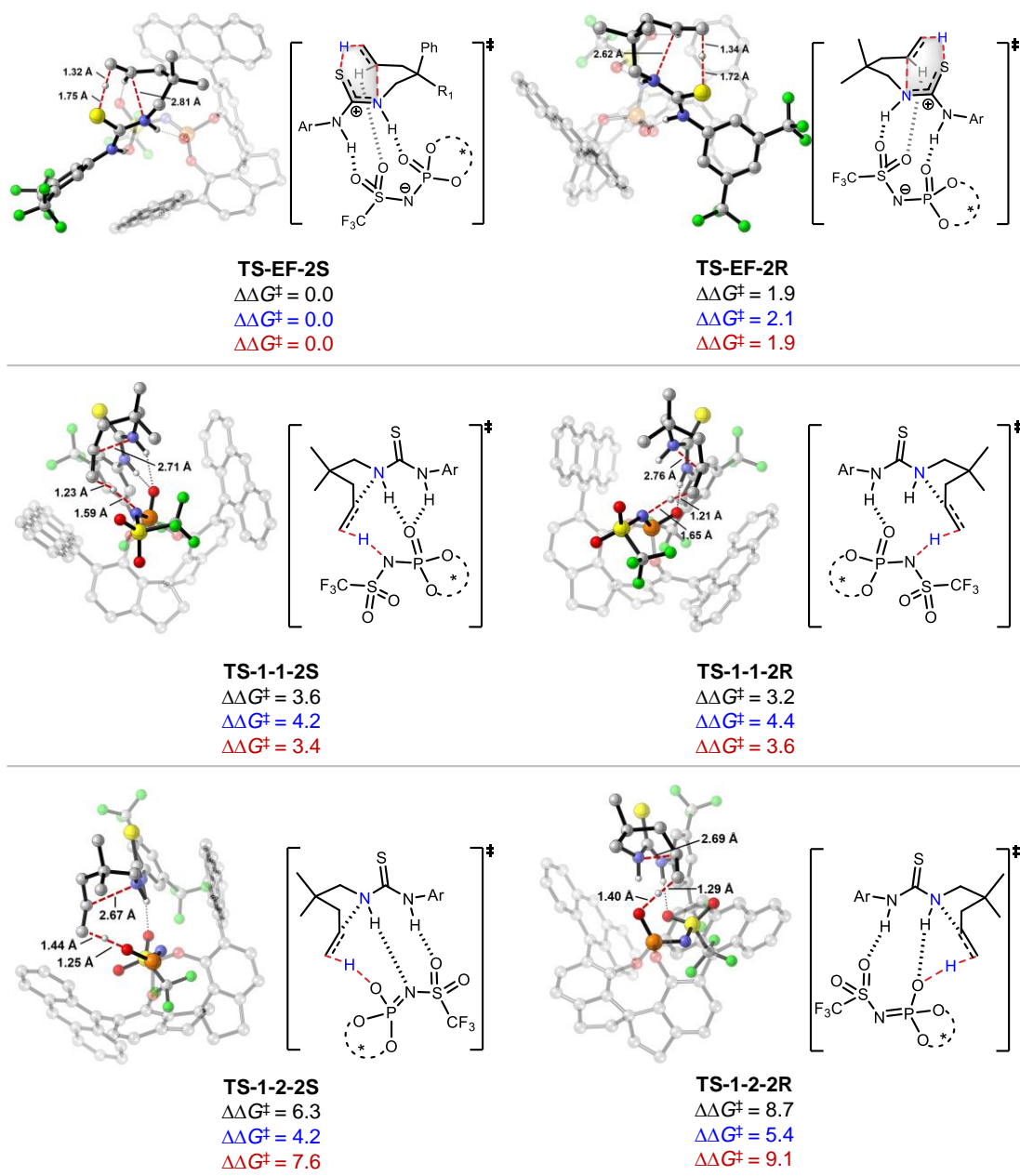


Fig. S10 Computed relative free energies of precomplexes along different reactions pathways of the reaction of **AT-2** catalyzed by **NTPA-2R** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to **INT-7**.



SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d)
SMD(DCM)- ω B97X-D/6-311+G(d,p)//B3LYP/6-31G(d)
SMD(DCM)-B3LYP-D3(BJ)/6-311+G(d,p)//B3LYP/6-31G(d)

Fig. S11 Computed favorable transition states of the reaction of **AT-2** catalyzed by **NTPA-2R** with three methods. Relative free energies are referred to **TS-EF-2S**.

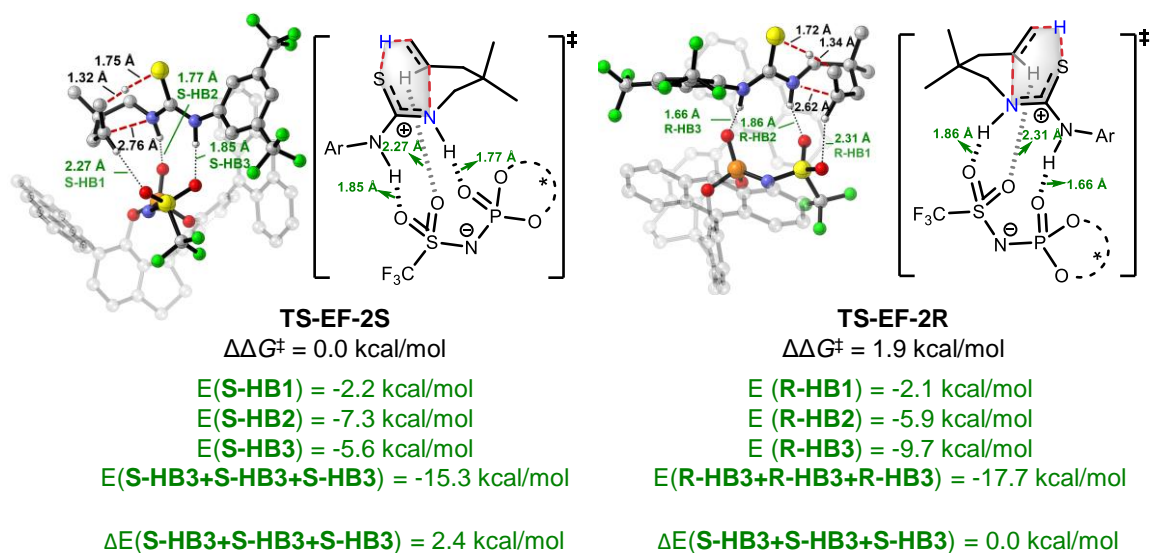


Fig. S12 Comparison of the hydrogen bond interactions in **TS-EF-2S** and **TS-EF-2R**.

1.4 The reaction of **AT-3** catalyzed by **NTPA-2R**

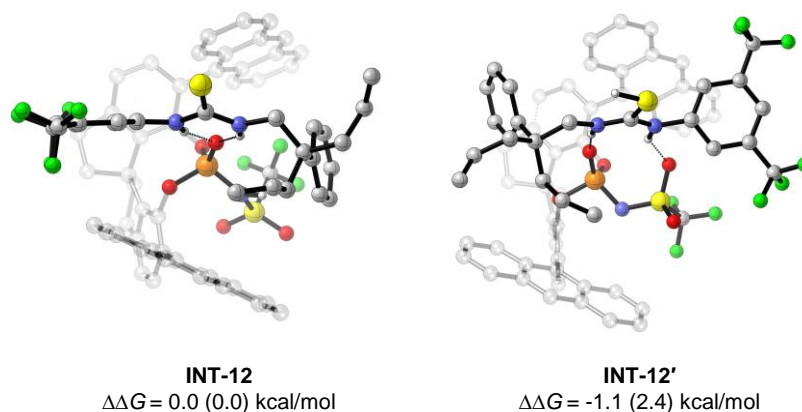


Fig. S13 Computed relative free energies of precomplexes along different reactions pathways for the reaction of **AT-3** catalyzed by **NTPA-2R** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Energies in cyclohexane were also calculated at the SMD(cyclohexane)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level and shown in parenthesis. Relative free energies are referred to **INT-12**.

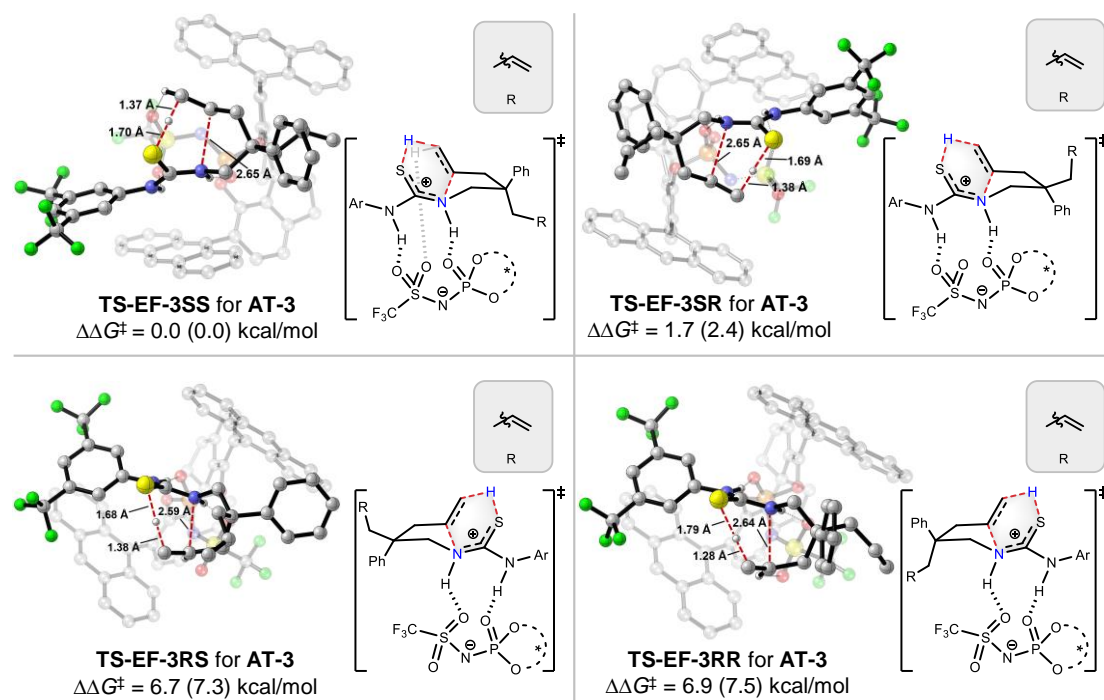


Fig. S14 Geometries and energies of the four optimized hetero-ene transition states leading to the four product stereoisomers of **AT-3** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Energies in cyclohexane were also calculated at the SMD(cyclohexane)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level and shown in parenthesis. Relative free energies are referred to **TS-EF-3SS**.

1.5 The reaction of **AT-4** catalyzed by **NTPA-2R**

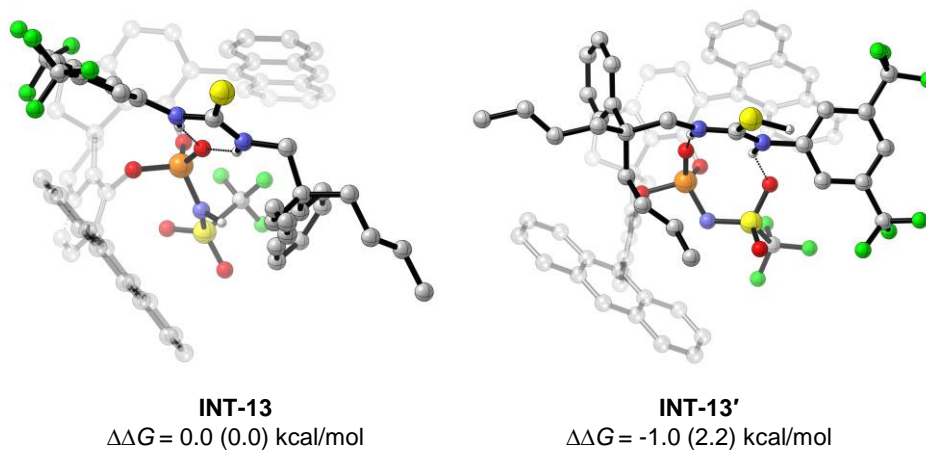


Fig. S15 Computed relative free energies of precomplexes along different reactions pathways for the reaction of **AT-4** catalyzed by **NTPA-2R** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Energies in cyclohexane were also calculated at the SMD(cyclohexane)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level and shown in parenthesis. Relative free energies are referred to **INT-13**.

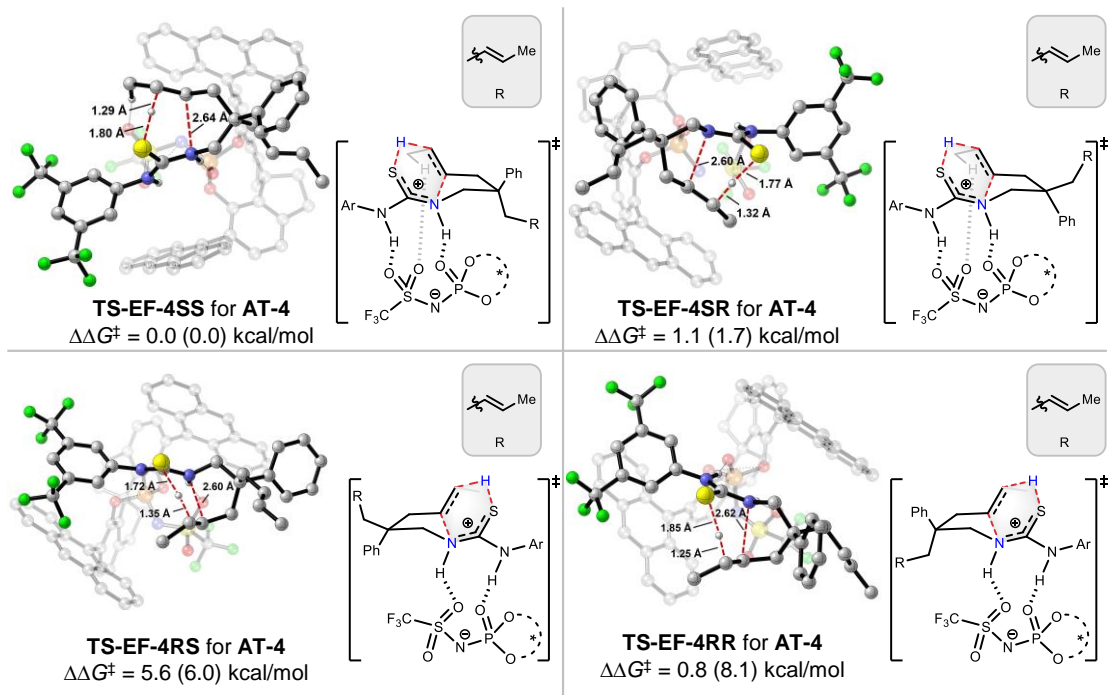


Fig. S16 Geometries and energies of the four optimized hetero-ene transition states leading to the four product stereoisomers of **AT-4** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Energies in cyclohexane were also calculated at the SMD(cyclohexane)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level and shown in parenthesis. Relative free energies are referred to **TS-EF-4SS**.

1.6 The reaction of **AT-5** catalyzed by **NTPA-2R**

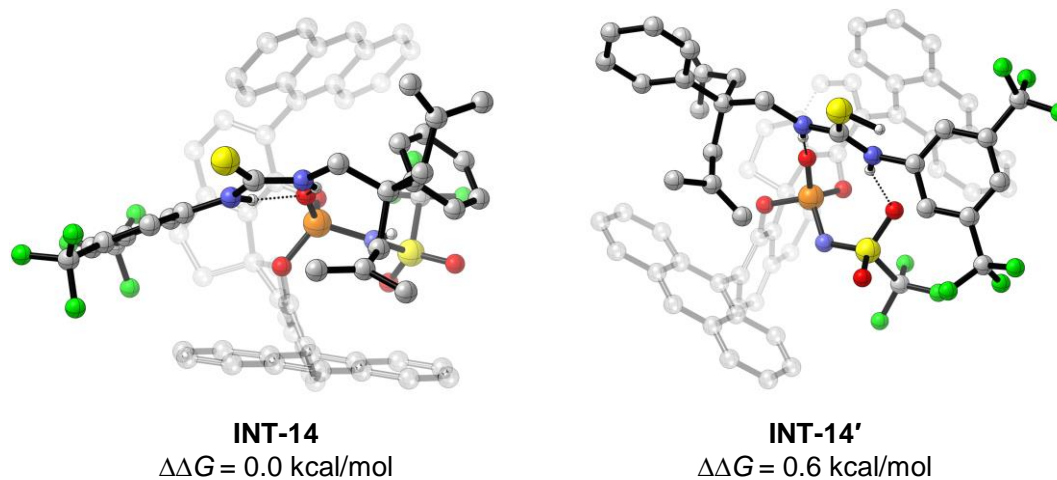


Fig. S17 Computed relative free energies of precomplexes along different reactions pathways for the reaction of **AT-5** catalyzed by **NTPA-2R** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to **INT-14**.

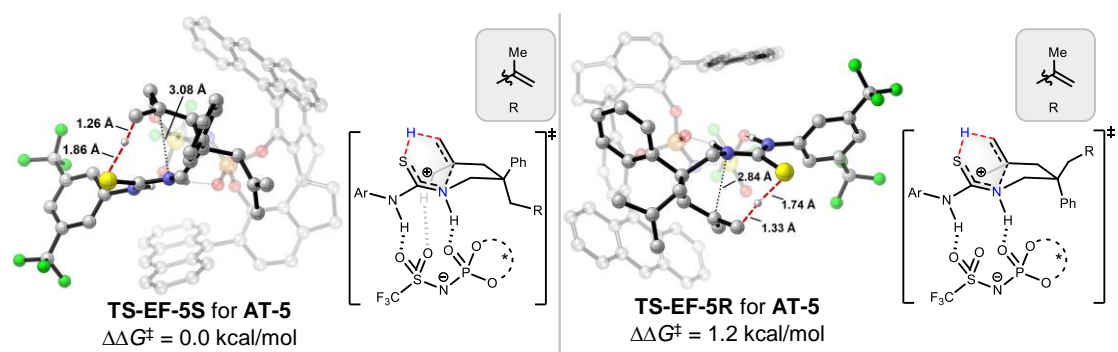


Fig. S18 Geometries and energies of the two optimized hetero-ene transition states leading to the two product enantiomers of **AT-5** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to **TS-EF-5S**.

1.7 The reaction of **AT-6** catalyzed by **NTPA-2R**

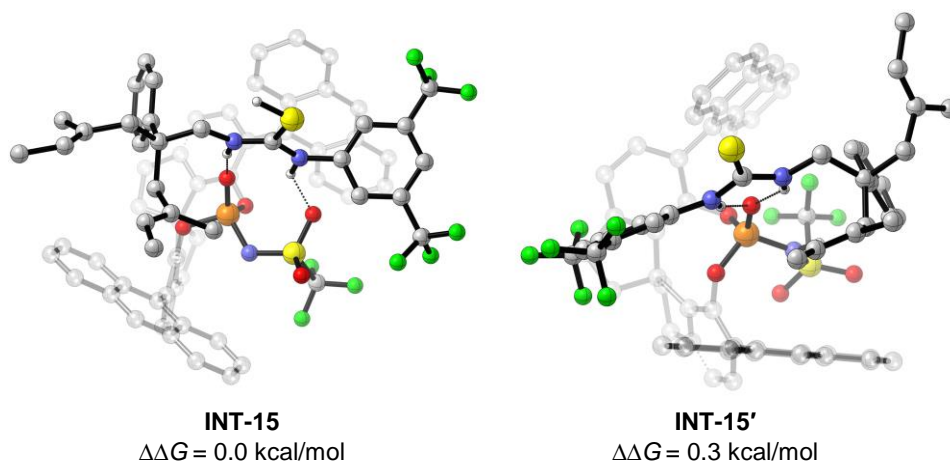


Fig. S19 Computed relative free energies of precomplexes along different reactions pathways for the reaction of **AT-6** catalyzed by **NTPA-2R** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are compared to **INT-15**.

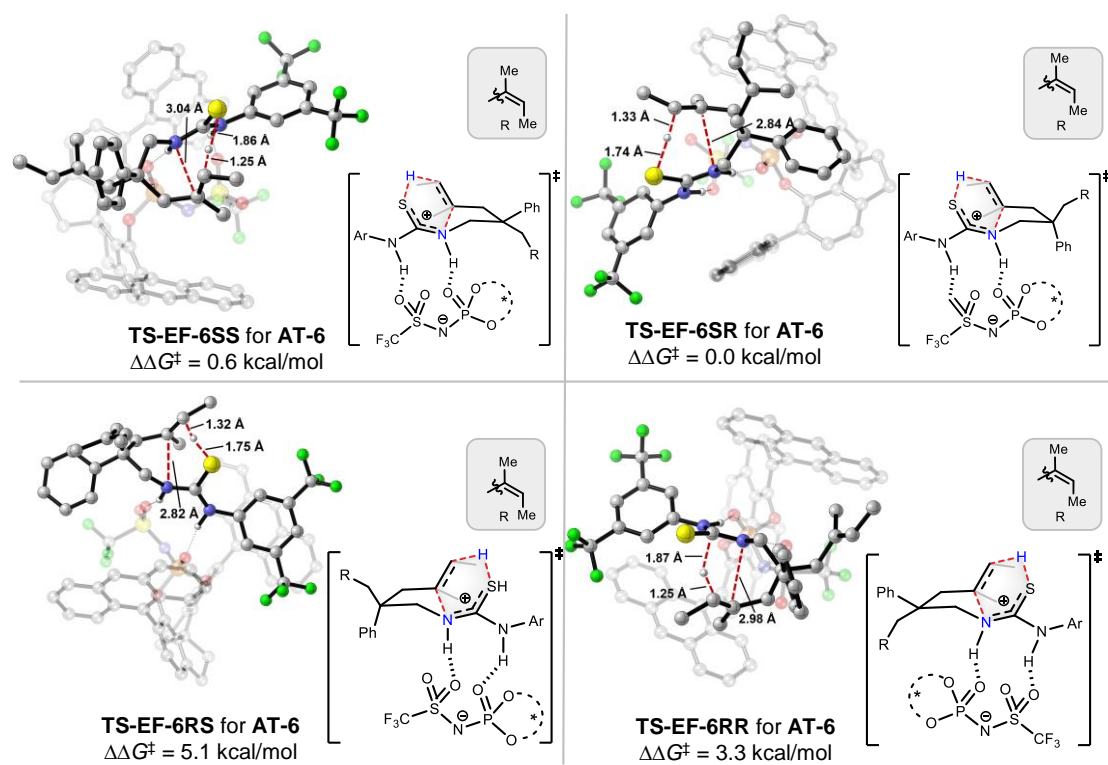


Fig. S20 Geometries and energies of the four optimized hetero-ene transition states leading to the four product stereoisomers of **AT-6** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to **TS-EF-6SR**.

1.8 The reaction of **AT-7** catalyzed by **NTPA-2R**

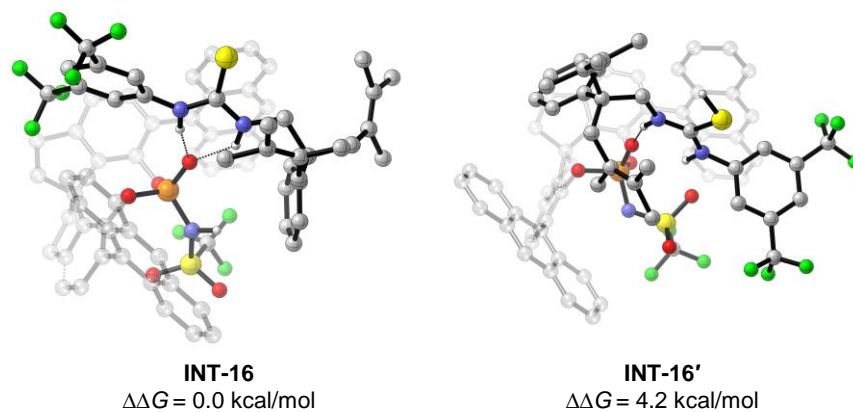


Fig. S21 Computed relative free energies of precomplexes along different reactions pathways for the reaction of **AT-7** catalyzed by **NTPA-2R** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to **INT-16**.

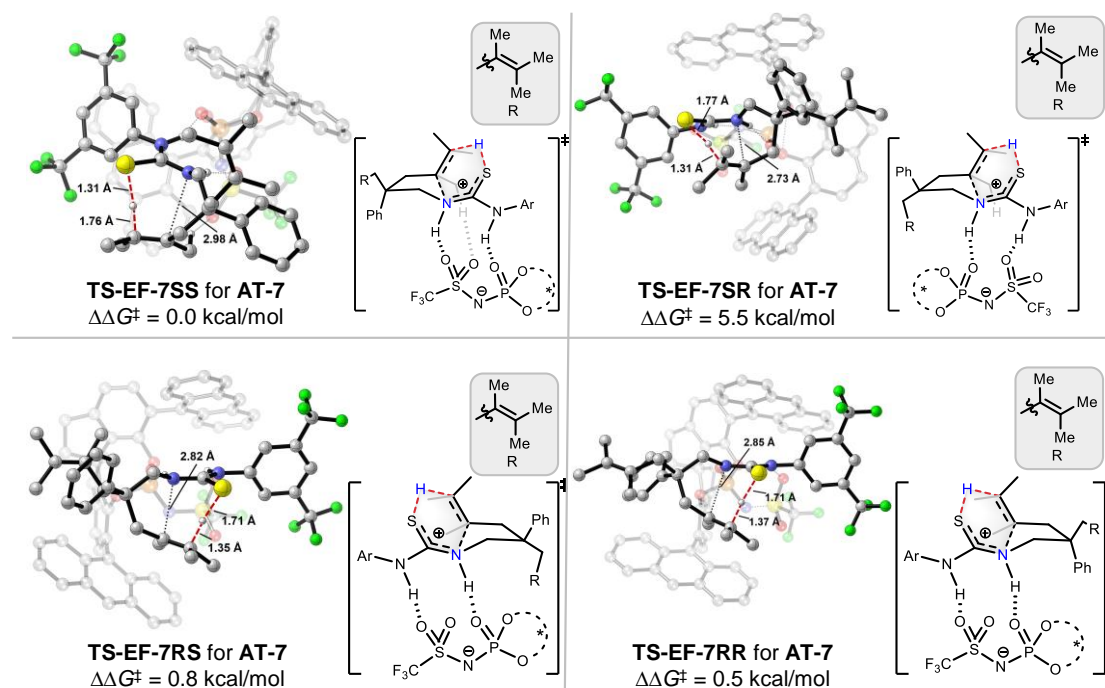


Fig. S22 Geometries and energies of the four optimized hetero-ene transition states leading to the four product stereoisomers of **AT-7** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to **TS-EF-7SS**.

1.9 Summary of computational results on different substituted alkenes

Table S2. Computational Results of Different Substituted Alkenes

Compd. No.	NPA charge in S.M.		NPA charge in T.S.		Length in T.S. (Å)			Reaction barrier ΔG (kcal/mol)
	C1	C2	C1'	C2'	C1'-N	C2'-H	S-H	
AT-3	-0.21	-0.44	0.02	-0.67	2.65	1.37	1.70	18.5 (19.1)
AT-4	-0.22	-0.22	0.05	-0.49	2.64	1.29	1.80	20.8 (22.7)
AT-5	-0.01	-0.44	0.31	-0.73	3.08	1.26	1.86	14.4
AT-6	-0.02	-0.22	0.25	-0.48	2.84	1.33	1.74	15.0
AT-7	-0.02	-0.02	0.25	-0.27	2.98	1.31	1.76	16.7

1.10 The reaction of **AT-1** catalyzed by **CPA-1R**

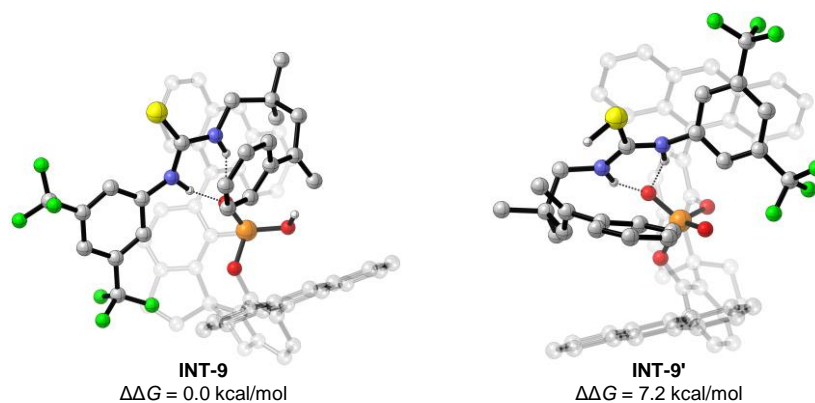


Fig. S23 Computed relative free energies of precomplexes along different reactions pathways for the reaction of **AT-1** catalyzed by **CPA-1R** at the SMD(DCM)-M06-2X/6-311+G(d,p)//B3LYP/6-31G(d) theory level. Relative free energies are referred to **INT-9**.

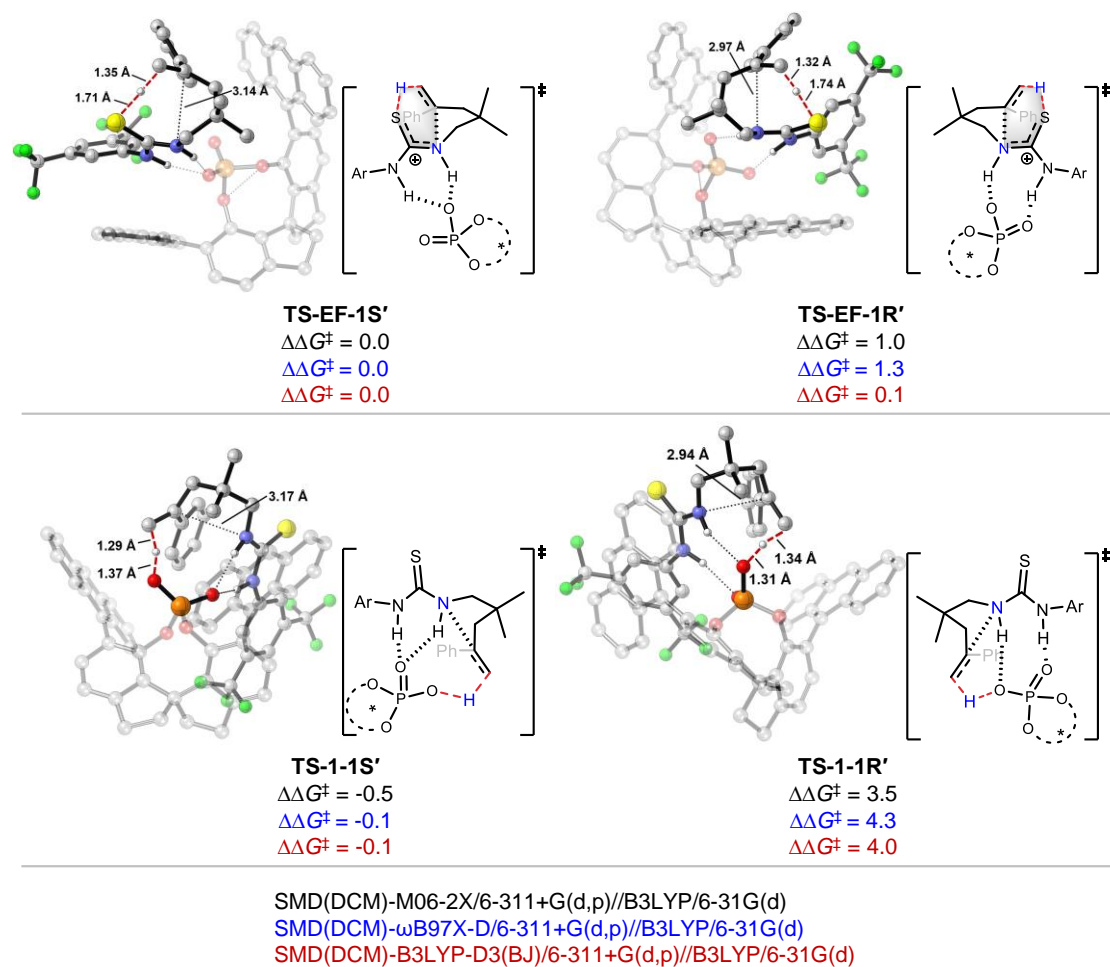


Fig. S24 Computed favorable transition states of the reaction of **AT-1** catalyzed by **CPA-1R** with three methods. Relative free energies are referred to **TS-EF-1S'**.

2. Energies and Cartesian coordinates of DFT-computed structures

NTPA-1

0 imaginary frequency

H = -1588.293608

G = -1588.357204

E(M06-2X-DCM) = -1588.420716

O	1.26938300	1.55015600	0.00561600
O	2.08087200	-0.58986000	-0.90336500
P	1.67529800	0.08145300	0.48725500
O	2.60807300	-0.06646300	1.62378600
N	0.15717000	-0.57166500	0.93228900
H	0.03583300	-0.74039500	1.92792400
S	-1.21032400	-0.95104400	0.04382200
C	-2.11465200	0.68701700	-0.11558600
O	-2.03708100	-1.77873400	0.91298800
O	-0.82212800	-1.33987600	-1.30333100
F	-3.34432500	0.43442300	-0.56178800
F	-2.18444700	1.27237400	1.08118100
F	-1.48385700	1.48518500	-0.97086400
C	2.52082200	-1.96500700	-0.95325500
H	3.22098700	-2.17382800	-0.14011900
H	1.65167800	-2.62478900	-0.89774700
H	3.01687800	-2.08870800	-1.91637100
C	2.26686700	2.41040100	-0.58712000
H	1.78252200	3.37668100	-0.72994300
H	3.12357600	2.51918400	0.08395400
H	2.58653700	2.00435700	-1.55025100

NTPA-1'

0 imaginary frequency

H = -1588.274310

G = -1588.340037

E(M06-2X-DCM) = -1588.411007

O	-2.59178400	-0.95511900	0.09328500
O	-1.49321700	1.23766300	-0.64836100
P	-1.50161400	0.13719000	0.50109100
N	-0.07221300	-0.36073200	0.93003100
S	1.14628600	-0.86822700	-0.01712600
C	2.22934700	0.65462600	-0.06693300
O	0.72003900	-1.09526600	-1.40594000

O	1.92345300	-1.88278700	0.68653700
F	1.54259700	1.69175500	-0.56065100
F	2.65516000	0.96101900	1.16070600
F	3.28222100	0.41345900	-0.85039300
O	-2.19839700	0.81860600	1.77321200
H	-1.61784500	0.73576700	2.54959400
C	-2.70939800	1.84030800	-1.14689000
H	-3.17939900	2.43573900	-0.35959100
H	-2.40457800	2.48254300	-1.97293300
H	-3.39962300	1.07084600	-1.50175400
C	-2.24801200	-2.11736200	-0.70703700
H	-1.58183600	-2.76932800	-0.13771700
H	-3.19444000	-2.62147800	-0.90219000
H	-1.76532800	-1.82149600	-1.63964300

NTPA-1''

0 imaginary frequency

H = -1588.277547

G = -1588.339452

E(M06-2X-DCM) = -1588.401143

O	-2.72829000	-1.01929900	0.10716900
O	-1.80703100	1.27908000	-0.55690300
P	-1.47857400	-0.03958700	0.30057800
N	-0.20651300	-0.71725000	-0.50771100
S	1.20061800	-0.86377900	0.11259700
C	2.19104900	0.65350300	-0.35880800
O	1.98963400	-2.01450700	-0.28201300
O	1.17694400	-0.68627600	1.69471700
F	1.53560800	1.74076600	0.05756400
F	3.39107200	0.60856300	0.21115900
F	2.32040200	0.68947600	-1.68217300
O	-1.22359100	0.21038400	1.76152200
H	0.24861300	-0.30616300	1.95830400
C	-3.06062300	-1.55316000	-1.19211200
H	-2.23259900	-2.15692900	-1.57168700
H	-3.94441400	-2.17432400	-1.04334800
H	-3.28551000	-0.74450200	-1.89418300
C	-2.77088100	2.22097700	-0.03538000
H	-2.46828400	2.56079600	0.95823700
H	-2.78068600	3.05799000	-0.73422000
H	-3.76515800	1.76593400	0.01354800

NTPA-1''-1

0 imaginary frequency

H = -1588.256429

G = -1588.321577

E(M06-2X-DCM) = -1588.388744

O	-2.78629400	-1.01859000	0.11990600
O	-1.62086200	1.16140000	-0.59006900
P	-1.54209000	-0.06553300	0.46660300
N	-0.24373300	-0.91361300	-0.18444700
S	1.20819800	-0.85402500	0.22726400
C	1.97991100	0.78931300	-0.27216500
O	1.74033700	-1.16702700	1.55079300
F	1.49353800	1.73700800	0.52465900
F	3.30509600	0.71358200	-0.12882100
F	1.68219100	1.06339100	-1.53716500
O	-1.49552500	0.32440800	1.88873500
C	-2.97350500	-1.56468800	-1.19719100
H	-2.14786300	-2.23595400	-1.44951200
H	-3.91164900	-2.12087300	-1.16408500
H	-3.04005500	-0.76558200	-1.94212000
C	-2.45204800	2.28907200	-0.24731800
H	-2.19789300	2.66308200	0.74751000
H	-2.25420400	3.05233000	-1.00170100
H	-3.51055600	2.00951800	-0.27570500
O	1.93724900	-1.80833400	-0.87586300
H	2.71572300	-2.20271400	-0.43454400

NTPA-1''-2

0 imaginary frequency

H = -1588.255141

G = -1588.319820

E(M06-2X-DCM) = -1588.388967

O	-2.76773100	-0.92428800	0.11491800
O	-1.24702800	0.99991700	-0.69068200
P	-1.62453500	0.09322000	0.60348200
O	-2.02461800	0.83889500	1.80918000
N	-0.24911800	-0.85562200	0.73628600
S	1.04877500	-0.91170000	-0.02205300
C	1.94758300	0.75501600	-0.07649700
O	1.21801400	-1.48514800	-1.35875300
F	3.26393500	0.52091300	-0.12671500
F	1.57860500	1.42083300	-1.16314900
F	1.65699800	1.45660400	1.01236200
O	2.03750600	-1.69097100	1.01140800
H	2.74589900	-2.10614600	0.48068300
C	-1.97042300	2.22774200	-0.91388400

H	-2.03185700	2.80612200	0.01089500
H	-1.40865900	2.77711800	-1.67097100
H	-2.97794900	2.01254300	-1.28368300
C	-2.57580000	-1.78184600	-1.02178600
H	-1.73119700	-2.45731400	-0.85540000
H	-3.49595500	-2.35883300	-1.12502400
H	-2.40199400	-1.19308200	-1.92793600

NTPA-1''-3

0 imaginary frequency

H = -1588.266214

G = -1588.328206

E(M06-2X-DCM) = -1588.394693

O	2.75205000	0.67159000	0.87336600
O	1.63365500	-0.68384500	-1.02951200
P	1.47035400	-0.23127800	0.56146500
O	1.34739700	-1.38168000	1.47494200
N	0.23580200	0.87354600	0.42241800
S	-1.05210500	0.81271300	-0.39890700
C	-2.25301000	-0.41918700	0.35445300
O	-1.78290900	2.04965200	-0.59533200
F	-3.35917400	-0.47213100	-0.38121500
F	-1.67375900	-1.61895400	0.38733500
F	-2.54505100	-0.02239900	1.58772600
O	-0.81412300	0.07670500	-1.81824200
H	0.10509500	-0.31593000	-1.79209400
C	2.41433700	-1.87317700	-1.30763200
H	2.02560600	-2.71930200	-0.73764000
H	2.32783700	-2.05400600	-2.37998200
H	3.46057000	-1.69550100	-1.04500400
C	3.01295100	1.90421000	0.17542500
H	2.19048600	2.60706300	0.32875100
H	3.93399400	2.30119500	0.60405000
H	3.15178400	1.71830600	-0.89435400

NTPA-1'-1

0 imaginary frequency

H = -1588.284803

G = -1588.347318

E(M06-2X-DCM) = -1588.414184

O	-2.73092300	-0.96782900	0.05371400
O	-1.78299900	1.33704900	-0.52294800
P	-1.44187000	-0.04239300	0.20219200
N	-0.16515000	-0.69302600	-0.47925800

S	1.26076700	-0.84811300	0.24594600
C	2.20589000	0.63959600	-0.37032700
O	1.98020700	-2.01774300	-0.23506300
O	1.15238800	-0.61992800	1.71477900
F	1.54728900	1.75507900	-0.02200800
F	3.41795700	0.65691200	0.18369300
F	2.32407800	0.59809900	-1.69629300
O	-1.36218500	0.23098200	1.76037600
H	-0.45327600	-0.04218500	2.07980200
C	-2.98710400	-1.67669200	-1.18317700
H	-2.12418800	-2.29265300	-1.44412100
H	-3.85943800	-2.30054100	-0.98911000
H	-3.20325700	-0.96932500	-1.98920700
C	-2.88108500	2.16199800	-0.06677100
H	-2.69583000	2.49734100	0.95657700
H	-2.91149100	3.01568700	-0.74366800
H	-3.82273100	1.60809800	-0.11722300

NTPA-1' -2

0 imaginary frequency

H = -1588.284268

G = -1588.346514

E(M06-2X-DCM) = -1588.414337

O	1.75256500	1.40406500	0.48386200
O	2.71189700	-0.61373800	-0.76276800
P	1.45846100	-0.11433900	0.08079500
N	0.17385100	-0.30649100	-0.83098000
S	-1.20455000	-0.94461000	-0.31186100
C	-2.19117700	0.57615100	0.13701300
O	-1.02805600	-1.65336000	0.98665400
O	-1.93755800	-1.60175700	-1.38215700
F	-3.39559200	0.22756600	0.58181000
F	-1.54279500	1.25328100	1.10083000
F	-2.32229800	1.37464100	-0.92632400
O	1.46820600	-0.86738400	1.47491200
H	0.58095100	-1.31294100	1.59861600
C	4.04249700	-0.58968400	-0.19491100
H	4.09170800	-1.25723100	0.66893600
H	4.70598500	-0.94491000	-0.98311600
H	4.31625200	0.42768500	0.09798300
C	1.46449800	2.47640000	-0.44585000
H	0.40653300	2.46246100	-0.71501600
H	1.71084700	3.39701400	0.08306900
H	2.08150100	2.38300300	-1.34416200

NTPA-1-1

0 imaginary frequency

H = -1588.289452

G = -1588.352581

E(M06-2X-DCM) = -1588.418235

O	2.59667500	1.06737400	0.84353500
O	2.11461300	-0.86013000	-0.72125000
P	1.53926300	-0.09781900	0.55571500
O	1.18127300	-0.91415000	1.72836800
N	0.26188100	0.88150800	-0.09623100
H	0.16033400	1.81112500	0.30539200
S	-1.12055900	0.35792800	-0.87235000
C	-2.27287100	-0.10168700	0.53655500
O	-0.80723900	-0.87875400	-1.57486700
O	-1.72409900	1.51836400	-1.51251600
F	-1.83722100	-1.19599800	1.14801500
F	-2.31839800	0.91405200	1.40505100
F	-3.48832200	-0.31543400	0.03623600
C	1.98195000	-2.29554800	-0.87338100
H	1.07464600	-2.50103600	-1.44274400
H	2.86453300	-2.62436200	-1.42386600
H	1.93971000	-2.77938800	0.10433400
C	3.33895000	1.71718500	-0.21050100
H	2.66077800	2.17544000	-0.93704000
H	3.93790900	2.48672400	0.27755700
H	3.98644600	0.99646700	-0.71406300

NTPA-1-2

0 imaginary frequency

H = -1588.289569

G = -1588.353369

E(M06-2X-DCM) = -1588.419117

O	-2.65985700	-0.96603600	0.09918100
O	-1.30029700	1.08797600	-0.60620400
P	-1.67206600	0.16480700	0.65044600
O	-2.18540900	0.79491900	1.87938800
N	-0.13814200	-0.55314100	0.94718800
H	0.06091400	-0.69312200	1.93530700
S	1.16656000	-0.92798500	-0.02921100
C	2.15244400	0.66983900	-0.07955800
O	0.70004800	-1.18067300	-1.38465600
O	1.99152100	-1.86497300	0.72203900
F	3.34060300	0.40266100	-0.61874200

F	1.52896800	1.59123300	-0.80552900
F	2.31587500	1.11676000	1.16797000
C	-2.38503100	-1.79423200	-1.04968100
H	-1.60239400	-2.51875300	-0.81370600
H	-3.31963900	-2.31103700	-1.27115900
H	-2.07178100	-1.18988900	-1.90411600
C	-2.29236200	2.00577100	-1.11716600
H	-1.80164300	2.56258200	-1.91558200
H	-3.15131400	1.45833800	-1.51713900
H	-2.61849100	2.68565800	-0.32607900

NTPA-1-3

0 imaginary frequency

H = -1588.289569

G = -1588.353370

E(M06-2X-DCM) = -1588.419117

O	-2.65985800	-0.96603600	0.09918200
O	-1.30029700	1.08797500	-0.60620300
P	-1.67206600	0.16480700	0.65044700
O	-2.18540900	0.79491900	1.87938800
N	-0.13814200	-0.55314100	0.94718800
H	0.06091300	-0.69312800	1.93530700
S	1.16656100	-0.92798400	-0.02921200
C	2.15244500	0.66983900	-0.07955800
O	0.70004800	-1.18067300	-1.38465600
O	1.99152100	-1.86497300	0.72203900
F	3.34060400	0.40266000	-0.61874200
F	1.52896900	1.59123300	-0.80552900
F	2.31587500	1.11675900	1.16797100
C	-2.38503400	-1.79423000	-1.04968300
H	-1.60239300	-2.51874800	-0.81371200
H	-3.31964000	-2.31103700	-1.27115700
H	-2.07179000	-1.18988500	-1.90411900
C	-2.29236100	2.00577100	-1.11716600
H	-1.80164200	2.56258000	-1.91558400
H	-3.15131500	1.45834100	-1.51713600
H	-2.61848700	2.68566100	-0.32608000

AT-1

0 imaginary frequency

H = -1957.907268

G = -1958.004909

E(M06-2X-DCM) = -1958.255431

C	-4.19281100	1.94412900	-0.12929300
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C	-4.63871700	0.88114700	-1.19045500
H	-3.78084500	0.68163700	-1.84375600
H	-5.39354700	1.36117200	-1.82428800
C	-4.25485800	-1.56472700	-0.41593400
C	-3.26370800	-1.91250300	-1.35455800
C	-4.33232600	-2.32116000	0.76726300
C	-2.38578200	-2.97354100	-1.11637600
H	-3.19729400	-1.37029000	-2.29397100
C	-3.45512700	-3.37859800	1.00708200
H	-5.07744700	-2.05731200	1.51227900
C	-2.47460100	-3.70814900	0.06885900
H	-1.64536200	-3.23672200	-1.86767300
H	-3.53166300	-3.94013800	1.93415900
H	-1.79116800	-4.53167800	0.25581500
C	-5.19874700	-0.43416900	-0.66849000
C	-3.23616700	1.36264800	0.94226900
H	-2.89476100	2.16545500	1.59890000
H	-3.77641600	0.63218800	1.55817100
N	-2.04528900	0.71082400	0.41407800
C	-0.75394800	1.07487400	0.63444100
N	0.12244000	0.10731400	0.16416100
C	1.52723300	0.08128400	0.10518000
C	2.32619200	1.22204500	-0.05907800
C	2.13935600	-1.17940700	0.14409500
C	3.70944600	1.08215000	-0.16315100
C	3.52233100	-1.30072100	0.02804600
H	1.53297600	-2.07221200	0.26733300
C	4.32320500	-0.17005800	-0.12043700
H	5.39921700	-0.26184500	-0.20381800
C	4.15523200	-2.66259000	0.13887500
C	4.55476100	2.30639600	-0.41144600
F	3.34494000	-3.63132700	-0.34900000
F	5.32219700	-2.73088500	-0.53524000
F	4.42061100	-2.98708800	1.42460000
F	4.71177700	2.53369800	-1.73717700
F	4.00633900	3.41732600	0.11809500
F	5.79362000	2.17015700	0.11160800
S	-0.29210600	2.49895800	1.39422100
C	-5.42030700	2.49316400	0.62062600
H	-5.11923800	3.24683800	1.35771100
H	-5.96118600	1.70088600	1.14959000
H	-6.11903800	2.97150500	-0.07595800
C	-3.49796700	3.09182400	-0.88509900
H	-3.22312800	3.90161600	-0.20119700

H	-4.15956700	3.50605600	-1.65570600
H	-2.58017200	2.74847100	-1.37432400
H	1.87159800	2.20138400	-0.09259400
C	-6.51227300	-0.59891800	-0.44916400
H	-0.29888900	-0.79489500	-0.02975500
H	-7.22286700	0.20170500	-0.63530700
H	-6.92309500	-1.54301700	-0.10227600
H	-2.21231000	-0.17874500	-0.04406700

AT-1-1

0 imaginary frequency

H = -1957.905743

G = -1958.001927

E(M06-2X-DCM) = -1958.254488

C	-4.28173500	-1.64878600	0.60346700
C	-5.10351200	-0.63638400	-0.26508200
H	-5.77032200	-0.09153900	0.41683200
H	-5.76389900	-1.22594400	-0.91201700
C	-3.67404700	1.53985900	-0.59075800
C	-4.14019800	2.18953500	0.56461300
C	-2.52301700	2.06466700	-1.21289300
C	-3.49083000	3.31503500	1.07239800
H	-5.02826100	1.82315100	1.06894200
C	-1.87108300	3.18912900	-0.70579500
H	-2.13969800	1.59151400	-2.11438500
C	-2.35186100	3.81936900	0.44404900
H	-3.87904300	3.79898600	1.96438500
H	-0.98973300	3.57475200	-1.21192800
H	-1.84377800	4.69185800	0.84427200
C	-4.38081100	0.35706900	-1.16741300
C	-3.21931000	-2.40685500	-0.23894600
H	-2.83231900	-3.25486800	0.32998300
H	-3.68441300	-2.80273100	-1.15129000
N	-2.06976500	-1.60207400	-0.62220800
C	-0.81389300	-1.68972100	-0.10844200
N	-0.05589700	-0.58117300	-0.46754400
C	1.31158500	-0.32977800	-0.25721100
C	2.29708000	-1.32025100	-0.37305800
C	1.69560400	0.99129600	0.00414400
C	3.63770100	-0.97812500	-0.20687400
C	3.04314000	1.31933400	0.14817900
H	0.93897200	1.76342200	0.10921700
C	4.02666800	0.33749900	0.05175700
H	5.07299200	0.59045000	0.17125200

C	3.43200200	2.75928700	0.35160800
C	4.68724800	-2.05906900	-0.26714800
F	3.56690400	3.40841000	-0.82963700
F	2.49909800	3.43580900	1.06076300
F	4.60652200	2.87898600	1.00378700
F	4.92782300	-2.58607900	0.95346000
F	4.31695100	-3.07623900	-1.07360700
F	5.86569700	-1.58211600	-0.72885700
S	-0.26422700	-2.95459500	0.84580200
C	-5.28345300	-2.70818300	1.11052100
H	-5.71589000	-3.28344600	0.28227100
H	-6.10952400	-2.23663600	1.65574700
H	-4.79288800	-3.41329200	1.79088500
C	-3.62002600	-0.97668500	1.81931700
H	-2.90526900	-0.20264800	1.53024200
H	-3.08098800	-1.71743200	2.41964500
H	-4.37811500	-0.50921000	2.45933200
H	2.01732300	-2.34123700	-0.59004600
C	-4.42286700	0.18373600	-2.50195800
H	-0.59894800	0.25627600	-0.65432000
H	-4.93494200	-0.66582800	-2.94533000
H	-3.98818700	0.89763500	-3.19545400
H	-2.25907600	-0.86779600	-1.29282300

AT-1-2

0 imaginary frequency

H = -1957.905743

G = -1958.001929

E(M06-2X-DCM) = -1958.254485

C	4.28162500	-1.64895500	-0.60364100
C	5.10344200	-0.63671500	0.26504800
H	5.77036200	-0.09187100	-0.41675500
H	5.76368300	-1.22641600	0.91200200
C	3.67424300	1.53970000	0.59076600
C	4.14073500	2.18959900	-0.56433200
C	2.52307000	2.06445500	1.21271200
C	3.49155600	3.31524300	-1.07206200
H	5.02892100	1.82330100	-1.06850500
C	1.87134300	3.18905400	0.70568100
H	2.13947100	1.59111200	2.11398100
C	2.35245400	3.81950500	-0.44391800
H	3.88004300	3.79935000	-1.96384500
H	0.98987900	3.57462600	1.21165200
H	1.84451400	4.69210100	-0.84409000

C	4.38073800	0.35673200	1.16738300
C	3.21913700	-2.40705900	0.23865600
H	2.83207900	-3.25493400	-0.33043600
H	3.68422500	-2.80314700	1.15091900
N	2.06967200	-1.60222700	0.62204000
C	0.81365600	-1.68999300	0.10863600
N	0.05569300	-0.58147100	0.46820300
C	-1.31172400	-0.32988900	0.25762600
C	-2.29738500	-1.32018800	0.37323300
C	-1.69552800	0.99128300	-0.00371900
C	-3.63796200	-0.97783700	0.20680000
C	-3.04295100	1.31952100	-0.14803900
H	-0.93876700	1.76331900	-0.10853100
C	-4.02667100	0.33781300	-0.05187000
H	-5.07292800	0.59093700	-0.17158400
C	-3.43156900	2.75951300	-0.35166500
C	-4.68756400	-2.05873500	0.26691500
F	-3.56669100	3.40874000	0.82950400
F	-2.49840700	3.43586500	-1.06062700
F	-4.60591300	2.87932200	-1.00414700
F	-4.31747800	-3.07576300	1.07371400
F	-5.86613200	-1.58171200	0.72820900
F	-4.92777000	-2.58603900	-0.95362100
S	0.26381800	-2.95483800	-0.84547200
C	5.28326300	-2.70836100	-1.11084500
H	5.71572200	-3.28371400	-0.28267000
H	6.10932700	-2.23681000	-1.65607900
H	4.79263300	-3.41339500	-1.79123900
C	3.61992900	-0.97665500	-1.81938700
H	2.90513100	-0.20269900	-1.53019900
H	3.08094800	-1.71732300	-2.41986700
H	4.37801400	-0.50903500	-2.45929900
H	-2.01786500	-2.34123100	0.59024200
C	4.42243800	0.18314500	2.50190500
H	0.59891500	0.25606300	0.65413400
H	4.93424100	-0.66660500	2.94523500
H	3.98767400	0.89696700	3.19542600
H	2.25901400	-0.86806300	1.29277400

AT-1-3

0 imaginary frequency

H = -1957.907362

G = -1958.004781

E(M06-2X-DCM) = -1958.255547

C	4.18911600	-1.94840100	-0.12835700
C	4.64776000	-0.88352500	-1.18210900
H	3.79594300	-0.67820700	-1.84152000
H	5.40568600	-1.36438100	-1.81161000
C	4.26757400	1.56093500	-0.40139800
C	3.28520500	1.91630700	-1.34637500
C	4.33875300	2.31237600	0.78534700
C	2.40958800	2.97982400	-1.11084800
H	3.22405300	1.37802700	-2.28840700
C	3.46381700	3.37229800	1.02250500
H	5.07700600	2.04267600	1.53508800
C	2.49196400	3.70937300	0.07796700
H	1.67606100	3.24885800	-1.86681700
H	3.53526600	3.92987000	1.95237700
H	1.81026200	4.53480100	0.26286100
C	5.20895500	0.42762300	-0.65106000
C	3.22584300	-1.36694100	0.93725000
H	2.87614900	-2.17058900	1.58847300
H	3.76360100	-0.64041700	1.55992300
N	2.04160100	-0.70915100	0.40150400
C	0.74744000	-1.06974800	0.60952700
N	-0.12240500	-0.09875400	0.13342800
C	-1.52726300	-0.07201700	0.07275600
C	-2.32158100	-1.21053200	-0.12481300
C	-2.14249400	1.18584200	0.13632800
C	-3.70472600	-1.07244100	-0.23396600
C	-3.52477000	1.30652600	0.01026200
H	-1.53873400	2.07720600	0.28082000
C	-4.32145200	0.17736400	-0.16973200
H	-5.39529500	0.27023900	-0.27567400
C	-4.16111200	2.66570500	0.13426100
C	-4.55482600	-2.30834300	-0.39171200
F	-5.32171100	2.74171000	-0.54994800
F	-4.43922200	2.97131400	1.42189800
F	-3.34806400	3.64285600	-0.33188500
F	-4.92813200	-2.80875500	0.80656100
F	-5.68912800	-2.04685700	-1.08011000
F	-3.89979100	-3.29033400	-1.04600900
S	0.27343100	-2.49395700	1.36137900
C	5.40826900	-2.50471100	0.62978400
H	5.09822700	-3.25985700	1.36161800
H	5.94772300	-1.71640800	1.16609400
H	6.11097900	-2.98322000	-0.06266900
C	3.49619800	-3.09087600	-0.89377600

H	2.58383200	-2.74236800	-1.38945700
H	3.21255800	-3.90186000	-0.21489900
H	4.16260400	-3.50510600	-1.66023000
H	-1.86258200	-2.18577100	-0.19501500
C	6.52141200	0.58644800	-0.42127900
H	0.30110100	0.80462600	-0.04998600
H	7.23026200	-0.21626700	-0.60505200
H	6.93324100	1.52765100	-0.06778700
H	2.21521200	0.18121200	-0.05265400

AT-1-4

0 imaginary frequency

H = -1957.905640

G = -1958.001950

E(M06-2X-DCM) = -1958.254282

C	4.29812000	-1.62760600	-0.59376100
C	5.09157100	-0.60903100	0.29386200
H	5.76174000	-0.05168600	-0.37452200
H	5.74948100	-1.19326500	0.94814900
C	3.62962400	1.54772800	0.60733100
C	4.10761700	2.21053200	-0.53569100
C	2.46042700	2.05326800	1.21145800
C	3.45190900	3.32983000	-1.04896600
H	5.00982800	1.85952900	-1.02567100
C	1.80101400	3.17062400	0.69791700
H	2.06824900	1.57022500	2.10392400
C	2.29405700	3.81387200	-0.43945700
H	3.84965800	3.82448300	-1.93082400
H	0.90278900	3.53932800	1.18688400
H	1.78057800	4.68083200	-0.84477900
C	4.34221900	0.37103800	1.18955400
C	3.24005100	-2.41348100	0.22863400
H	2.86934600	-3.25815500	-0.35600700
H	3.70383500	-2.81679300	1.13839900
N	2.07730400	-1.62994800	0.61504800
C	0.82750700	-1.72015300	0.08575500
N	0.06251800	-0.61758800	0.44536700
C	-1.30329400	-0.35880100	0.23720000
C	-2.29456900	-1.34887100	0.29352200
C	-1.68010500	0.97617000	0.04274800
C	-3.63257200	-0.98914500	0.14238200
C	-3.02399800	1.31945900	-0.09285200
H	-0.91949600	1.74992600	-0.00547300
C	-4.01377500	0.33992400	-0.05096200

H	-5.05819800	0.60413500	-0.16328800
C	-3.39117900	2.75543100	-0.35674100
C	-4.69981600	-2.04617100	0.27528400
F	-4.63698500	3.04460200	0.07331600
F	-2.53885600	3.60929000	0.26023500
F	-3.34849400	3.04982000	-1.67589000
F	-5.78212000	-1.75865900	-0.48158100
F	-4.25579300	-3.26464000	-0.09080100
F	-5.13281600	-2.14894300	1.55447800
S	0.29628600	-2.98010800	-0.88504400
C	5.32479200	-2.66346800	-1.09951200
H	4.85433300	-3.37224100	-1.79020400
H	5.76036100	-3.23718400	-0.27184200
H	6.14676000	-2.17184100	-1.63306300
C	3.63803900	-0.95555000	-1.81052000
H	4.39425100	-0.46628600	-2.43627900
H	2.90459100	-0.19888100	-1.52229400
H	3.12109800	-1.70027200	-2.42520100
H	-2.02076000	-2.38327100	0.44485600
C	4.36656700	0.19277400	2.52393900
H	0.60321400	0.21702400	0.65040800
H	4.88252300	-0.65215800	2.97169200
H	3.91269100	0.89856200	3.21346000
H	2.25413900	-0.90100900	1.29490500

TS-1-1

l imaginary frequency

H = -3546.192069

G = -3546.326390

E(M06-2X-DCM) = -3546.664642

O	0.89123100	-2.35789400	-0.36655600
O	2.86180100	-2.10834000	-2.00796800
P	1.95206200	-1.30089300	-0.96426000
O	1.16185000	-0.17461800	-1.55181900
N	2.98612800	-0.77190000	0.21503000
S	4.33291900	-1.49216800	0.79931400
C	5.69038800	-0.69844500	-0.21758200
F	6.87235300	-1.14519300	0.20746700
F	5.54687400	-0.98577600	-1.51135500
F	5.64302100	0.63360400	-0.06061500
C	1.98175800	3.88033600	-0.52491300
C	1.72893200	3.65254700	1.01475200
H	2.60969700	4.05797900	1.52729300
H	0.88611000	4.29294000	1.28067100

C	0.22212500	1.80280800	2.04795600
C	-0.83683500	2.69397000	2.32959300
C	-0.00287100	0.41978900	2.27067100
C	-2.04563800	2.22980400	2.84176500
H	-0.72111300	3.75879500	2.17392500
C	-1.22033700	-0.04142400	2.74851700
H	0.77180000	-0.29855500	2.02692200
C	-2.24348600	0.86622200	3.04974900
H	-2.84028200	2.93719900	3.05578100
H	-1.38834700	-1.10765700	2.86479400
H	-3.19519700	0.50570200	3.42922800
C	1.53056100	2.26245400	1.58084900
C	0.66949200	3.75549300	-1.33487900
H	0.89314800	4.00398700	-2.38396300
H	-0.06827300	4.48025700	-0.98375000
N	0.05690400	2.44574200	-1.26016700
C	-1.27742600	2.20142500	-1.12609300
N	-1.53914700	0.85008300	-1.20122300
C	-2.67668500	0.10704300	-0.85004500
C	-4.00061700	0.56206100	-0.94568200
C	-2.43912500	-1.20407100	-0.40705500
C	-5.04625300	-0.28179300	-0.56767800
C	-3.49660100	-2.02824600	-0.03158800
H	-1.41979600	-1.57319200	-0.34380700
C	-4.81373100	-1.57651600	-0.10180100
H	-5.63703500	-2.21861800	0.18519200
C	-3.17657200	-3.38356000	0.53480000
C	-6.45913200	0.24162200	-0.61335900
F	-2.21634200	-4.01934900	-0.18229600
F	-4.25093400	-4.19398700	0.57927700
F	-2.69702600	-3.29018700	1.80486500
F	-7.35552100	-0.75277000	-0.80554300
F	-6.63423600	1.14337700	-1.60092700
F	-6.79733300	0.85385900	0.54617800
S	-2.42402900	3.41332700	-0.87361000
C	2.44769400	5.34580400	-0.66800300
H	3.41280000	5.50128500	-0.17301400
H	2.56967600	5.60906900	-1.72466700
H	1.72421500	6.04394300	-0.23064800
C	3.07625900	2.96122100	-1.09635900
H	3.27580900	3.23378900	-2.13964400
H	4.01730000	3.06963300	-0.54564800
H	2.80256800	1.90335800	-1.08007100
H	-4.20330200	1.55948400	-1.30771400

C	2.65922700	1.43746900	1.74664600
H	-0.70238000	0.27225800	-1.30920300
H	3.62978900	1.90291900	1.58588700
H	2.65471200	0.76455200	2.60451300
O	4.38359800	-2.92487600	0.50921500
H	0.64868800	1.64489800	-1.47842300
O	4.55292500	-0.99476000	2.15812500
H	2.69425700	0.44167700	0.87947900
C	1.26137500	-3.60117900	0.27039000
H	1.74460000	-3.40692900	1.23083500
H	0.32484300	-4.13954300	0.41603600
H	1.94220500	-4.17377600	-0.36333200
C	2.28853800	-2.55008200	-3.25696000
H	1.89296200	-1.69703800	-3.81418400
H	3.10258000	-3.01844600	-3.81073600
H	1.49243400	-3.27939600	-3.07816300

TS-1-1-1

1 imaginary frequency

H = -3546.183571

G = -3546.319471

E(M06-2X-DCM) = -3546.656259

O	5.92818600	0.00067900	-1.07980300
O	5.16090900	-2.21068300	-0.01532200
P	5.06727200	-0.60530500	0.13704200
O	5.50976200	-0.02519100	1.42351200
N	3.43082100	-0.31331900	-0.12831700
S	2.36251800	-1.08538500	-1.03678100
C	1.86356500	-2.63682000	-0.08610600
F	0.61923300	-2.97991300	-0.44266000
F	2.68547900	-3.64320900	-0.35236200
F	1.88062600	-2.38997800	1.23372500
C	1.89888900	3.97001800	-0.29274100
C	1.75810400	3.63928200	1.24299600
H	2.68212500	3.99836100	1.70979300
H	0.95166800	4.27200200	1.61871200
C	0.25650500	1.72211300	2.14436900
C	-0.81964100	2.59263700	2.43009400
C	0.04025700	0.33132100	2.31986100
C	-2.03576600	2.10156900	2.89647800
H	-0.71464200	3.66307000	2.30930100
C	-1.18265400	-0.15651500	2.75563600
H	0.82414700	-0.37197200	2.07004100
C	-2.22359000	0.73000800	3.05836500

H	-2.84291700	2.79424000	3.11157600
H	-1.34134200	-1.22745200	2.83917700
H	-3.17977200	0.34762000	3.40355400
C	1.56878700	2.21535700	1.72470400
C	0.55630700	3.84361900	-1.04828000
H	0.71705200	4.18282600	-2.08327000
H	-0.19230100	4.50857400	-0.61230500
N	-0.01078200	2.50775500	-1.04882500
C	-1.34564900	2.22896700	-0.99856300
N	-1.58132000	0.87704100	-1.12360300
C	-2.72957100	0.11280600	-0.85233800
C	-4.04999300	0.54658600	-1.03866700
C	-2.49995800	-1.19521500	-0.39994900
C	-5.10421000	-0.31662000	-0.73526500
C	-3.56469500	-2.03906700	-0.09791000
H	-1.48179900	-1.54939200	-0.27682600
C	-4.88088100	-1.60814700	-0.25654200
H	-5.71033300	-2.26566100	-0.02786600
C	-3.25982900	-3.39061200	0.48773800
C	-6.51964600	0.18227900	-0.87854400
F	-2.21416300	-3.98393300	-0.12823600
F	-4.31054500	-4.23119500	0.41652700
F	-2.92292400	-3.28919500	1.80291400
F	-7.38280400	-0.82724000	-1.13164700
F	-6.64089300	1.08147300	-1.87662200
F	-6.94696400	0.78810900	0.25426800
S	-2.52754700	3.41072700	-0.78265200
C	2.29697500	5.46121100	-0.36614900
H	3.27359200	5.62907300	0.10104000
H	2.36636000	5.78967800	-1.40910500
H	1.56327700	6.10091700	0.13823600
C	3.00164900	3.14037600	-0.97248300
H	3.13796800	3.48238000	-2.00534400
H	3.96185200	3.25919800	-0.45765900
H	2.78199000	2.07093800	-1.00263200
H	-4.24508000	1.54102500	-1.41235000
C	2.71346900	1.40105800	1.84584200
H	-0.74043600	0.30560600	-1.16486600
H	3.67695300	1.90891300	1.82855400
H	2.67918200	0.60639100	2.59048300
O	2.85379500	-1.56684400	-2.32785700
H	0.61816600	1.73448600	-1.24730200
O	1.12821500	-0.26504400	-0.99991700
H	2.90082900	0.63226500	0.81013800

C	5.78585000	-0.41296600	-2.45133800
H	4.84620100	-0.04363800	-2.86775200
H	6.63215500	0.02424800	-2.98403600
H	5.80942800	-1.50249500	-2.53756400
C	6.35828400	-2.88297200	0.42547400
H	6.58603200	-2.61140300	1.45937500
H	6.15040300	-3.95116700	0.35113700
H	7.20392000	-2.62411800	-0.21988100

TS-1-2

l imaginary frequency

H = -3546.187819

G = -3546.322496

E(M06-2X-DCM) = -3546.663485

O	4.27518300	2.00852100	-0.93955100
O	4.91747600	0.97948300	1.34624300
P	3.71458600	1.16062000	0.30063200
O	3.38777600	-0.26859800	-0.19543700
N	2.58282000	2.00234500	1.05660400
S	1.13630700	2.30774600	0.45321400
C	1.19534600	4.13654100	0.07804700
F	0.02980200	4.50335600	-0.45903500
F	2.18164100	4.39695700	-0.78500600
F	1.40203900	4.82796400	1.20071500
C	2.74125000	-3.91922200	-1.21365400
C	2.06610300	-4.08114000	0.19298100
H	2.63195700	-4.86457300	0.71951100
H	1.06724700	-4.47390500	-0.00203700
C	0.66602600	-2.55133900	1.72318900
C	-0.37227600	-3.49970200	1.84952800
C	0.42871700	-1.23938600	2.19448800
C	-1.58290800	-3.15352500	2.44317900
H	-0.22775500	-4.52068000	1.51683600
C	-0.79739400	-0.88610100	2.74203700
H	1.18462500	-0.47031400	2.08090700
C	-1.80680400	-1.84526500	2.87594500
H	-2.36359600	-3.90172300	2.54297700
H	-0.96619000	0.14508300	3.03394300
H	-2.77341200	-1.56880500	3.28535800
C	1.96893100	-2.91426500	1.15381400
C	1.88103400	-3.01203400	-2.15555500
H	2.54516700	-2.56277300	-2.90489800
H	1.15599300	-3.63345400	-2.68269200
N	1.11130400	-1.94720500	-1.52784700

C	-0.26341900	-1.91412500	-1.52623000
N	-0.75587700	-0.68784300	-1.17597200
C	-2.07400300	-0.26887600	-0.89988100
C	-3.07374700	-1.10013700	-0.38120800
C	-2.34735900	1.09520500	-1.08362700
C	-4.31787300	-0.56035700	-0.05251200
C	-3.59528000	1.61512900	-0.75206700
H	-1.57189300	1.75085200	-1.46251000
C	-4.59637400	0.79347700	-0.23400800
H	-5.56489900	1.20026100	0.02953000
C	-3.87675600	3.07237100	-1.00777000
C	-5.33495500	-1.45190300	0.60733800
F	-2.76453100	3.82904200	-0.88934400
F	-4.35896600	3.27507200	-2.25696000
F	-4.79827700	3.56269900	-0.14897900
F	-6.59279900	-0.98216700	0.46943600
F	-5.30994000	-2.70714500	0.11402000
F	-5.10463500	-1.55921700	1.94551000
S	-1.20516200	-3.25930300	-1.92180900
H	-2.87972600	-2.15166100	-0.23153800
C	3.11605600	-2.21502600	1.54728300
H	-0.08475300	0.08223300	-1.11710800
H	4.07876100	-2.68196800	1.35580800
H	3.07047300	-1.65743700	2.48135800
O	0.91010700	1.67905000	-0.87720200
H	1.61193400	-1.08736100	-1.31514700
O	0.09618500	2.15297600	1.47211400
H	3.19879500	-1.19257100	0.65591600
C	2.75442700	-5.33189000	-1.84211500
H	3.42677400	-6.00354200	-1.29521600
H	1.75278200	-5.77541500	-1.85055400
H	3.10738500	-5.28359900	-2.87901700
C	4.20058100	-3.42176700	-1.16924800
H	4.80507700	-4.01092800	-0.46865900
H	4.65003600	-3.54387400	-2.16231600
H	4.28629100	-2.36629800	-0.90560000
C	5.19342900	1.42282900	-1.88445700
H	4.72080700	0.58370100	-2.40017400
H	5.43550400	2.21292500	-2.59607400
H	6.10389000	1.08563900	-1.37919700
C	5.35238600	2.08927900	2.16238000
H	4.51931100	2.46216000	2.76184400
H	6.14237200	1.69720700	2.80415600
H	5.74855100	2.89219500	1.53336000

TS-1-2-1

l imaginary frequency

H = -3546.175647

G = -3546.310796

E(M06-2X-DCM) = -3546.652195

O	4.94922100	-0.36401100	1.77044300
O	3.09886500	-1.72782700	2.93621400
P	3.35925300	-0.52372500	1.90533700
O	2.87188900	0.79959000	2.52485300
N	2.59440200	-1.02673700	0.58410300
S	2.86775200	-0.78253600	-0.95163100
C	2.96629800	-2.52951400	-1.60136500
F	3.23698200	-2.49758100	-2.90778800
F	3.94269200	-3.19356900	-0.96855600
F	1.80887000	-3.16690200	-1.40893200
C	1.19224700	4.51006000	-1.43986400
C	1.09048700	4.38633200	0.13583500
H	2.08895800	4.61986200	0.52912700
H	0.42891900	5.17529900	0.49899900
C	-0.59373100	2.89790800	1.40836400
C	-1.64953500	3.82109000	1.24789900
C	-0.81886600	1.77259000	2.23929100
C	-2.88192800	3.61349300	1.86198700
H	-1.53084300	4.68621600	0.60719500
C	-2.04783500	1.56966900	2.84937800
H	-0.01336500	1.06979900	2.42157500
C	-3.08856000	2.48636800	2.65641700
H	-3.68694000	4.32338000	1.69973500
H	-2.20396600	0.69485200	3.47286200
H	-4.05576500	2.31192700	3.11819200
C	0.68860600	3.05440700	0.72060800
C	-0.02560700	3.89252700	-2.17247500
H	0.08504800	4.09075600	-3.24898300
H	-0.95731400	4.37139500	-1.86284000
N	-0.18174900	2.46818000	-1.93048700
C	-1.37366500	1.81006000	-1.80522200
N	-1.18487600	0.47530600	-1.52851000
C	-2.07602700	-0.50306500	-1.05356200
C	-3.26318800	-0.21987800	-0.36771500
C	-1.67326400	-1.84165300	-1.19826200
C	-4.01963100	-1.26517300	0.16407400
C	-2.44778400	-2.87026800	-0.67044700
H	-0.73897900	-2.07174200	-1.69998600

C	-3.63098500	-2.59454900	0.01836300
H	-4.22532400	-3.39580800	0.43918600
C	-2.03311200	-4.30187900	-0.88967200
C	-5.22792600	-0.90857000	0.98844600
F	-2.42153900	-5.09579500	0.13347400
F	-0.69491200	-4.42812400	-1.01744500
F	-2.58704000	-4.81288000	-2.01364900
F	-4.86297800	-0.39042200	2.19367800
F	-6.01106400	-1.97707500	1.24346100
F	-5.99322400	0.02616600	0.38827200
S	-2.86152900	2.57744300	-1.98362700
C	1.19200200	6.02223300	-1.75190300
H	2.03036200	6.52298800	-1.25443800
H	1.29284400	6.19659400	-2.82887300
H	0.26444400	6.50245200	-1.41901800
C	2.50788800	3.92003600	-1.99252500
H	2.59676200	4.15684400	-3.05917400
H	3.37578400	4.35598600	-1.48431700
H	2.59001800	2.83347400	-1.90123500
H	-3.58429200	0.80431800	-0.24369100
C	1.57771800	1.97670700	0.62759700
H	-0.22504000	0.13480900	-1.60166600
H	1.10977500	1.00233100	0.49690100
H	2.44214200	2.12663000	-0.01530600
O	4.15093900	-0.14484300	-1.28753100
H	0.65755100	1.89716500	-1.96100500
O	1.66818200	-0.23995900	-1.64289100
H	2.19855400	1.56269800	1.72192600
C	5.78203500	-1.42605300	1.25509000
H	5.73544200	-1.42883200	0.16532100
H	6.79577900	-1.19715500	1.58729900
H	5.47199900	-2.39598500	1.65524000
C	3.36075800	-1.52524100	4.33927300
H	2.74719600	-0.70830700	4.72700800
H	3.09691100	-2.46237900	4.83104800
H	4.41933000	-1.30323200	4.50825200

TS-1-2-2

l imaginary frequency

H = -3546.185483

G = -3546.316633

E(M06-2X-DCM) = -3546.657946

O	3.01961900	-1.75551400	2.53494100
O	0.82943600	-1.78801200	1.36961200

P	2.07536300	-0.82590400	1.62300900
O	1.69112400	0.42001100	2.44429300
N	2.75016000	-0.39877900	0.23096100
S	2.98942300	-1.22221000	-1.12466200
C	4.12312700	-2.64878600	-0.69118300
F	4.48630600	-3.28116000	-1.80502200
F	5.21973400	-2.18874800	-0.07036000
F	3.49868700	-3.50770900	0.12173800
C	2.50984900	3.73893700	-0.97106900
C	1.53876200	4.38784900	0.08209500
H	2.12550300	5.15652100	0.60416300
H	0.77436100	4.90402100	-0.50010700
C	-0.57622700	3.45118300	1.23693600
C	-1.42944000	4.40701000	0.64509100
C	-1.17252400	2.38075100	1.94684700
C	-2.81229700	4.31377800	0.78115000
H	-1.02005400	5.25286900	0.10660500
C	-2.55277400	2.27099200	2.04446100
H	-0.54665900	1.60564500	2.37533500
C	-3.37995000	3.24268100	1.46927100
H	-3.44590900	5.06936600	0.32691900
H	-2.99502800	1.41839200	2.54955800
H	-4.45860400	3.14201000	1.53797600
C	0.88512900	3.56336000	1.16880000
C	1.72806600	2.84675600	-1.96241200
H	2.44327200	2.42656100	-2.68319900
H	1.00079000	3.44463800	-2.51497900
N	0.99341000	1.75601100	-1.34208300
C	-0.28432900	1.39234300	-1.66538200
N	-0.54932100	0.09175500	-1.27923400
C	-1.76201000	-0.55495900	-1.01514600
C	-2.96715700	0.10936500	-0.74625500
C	-1.72470300	-1.95764400	-0.93204500
C	-4.09622200	-0.62489300	-0.38382100
C	-2.86530700	-2.67040700	-0.57131500
H	-0.79654100	-2.48039100	-1.14069100
C	-4.06591900	-2.01568200	-0.29226400
H	-4.95202400	-2.57475800	-0.01890200
C	-2.77066500	-4.16175700	-0.39982100
C	-5.34253000	0.12200300	0.00828500
F	-1.90595000	-4.72354300	-1.26683100
F	-3.96460500	-4.77017200	-0.55459500
F	-2.33173300	-4.48482700	0.85087100
F	-6.45466200	-0.62937300	-0.12319100

F	-5.51785800	1.24699800	-0.71492900
F	-5.29126800	0.51296200	1.31550200
S	-1.37084300	2.41102000	-2.44696100
C	3.08754300	4.90967400	-1.79696200
H	3.70708800	5.56339100	-1.17242500
H	3.71905600	4.52926600	-2.60744800
H	2.29482300	5.51891500	-2.24704700
C	3.68395700	2.97466400	-0.33461100
H	4.36387700	2.62537700	-1.11940000
H	4.25637400	3.62741700	0.33652200
H	3.37349100	2.08909300	0.22313200
H	-3.01931700	1.18523300	-0.82241200
C	1.66723400	2.99458800	2.18750800
H	0.25494200	-0.53798700	-1.26980500
H	2.71661900	3.27784800	2.21949900
H	1.19859100	2.93726200	3.17124700
O	3.75684600	-0.38173000	-2.04526900
H	1.56228600	1.06834800	-0.85093900
O	1.75243600	-1.86396300	-1.61656800
H	1.70234400	1.64359800	2.08722300
C	4.25507900	-1.23240300	3.06078100
H	4.06817100	-0.32406400	3.64075900
H	4.66124200	-2.01031500	3.70851500
H	4.95232500	-1.02716800	2.24459300
C	0.12305200	-2.43046600	2.45607900
H	-0.30009400	-1.67765100	3.12730800
H	-0.67251400	-3.01170600	1.99171100
H	0.80210100	-3.08685300	3.00478100

TS-1-2-3

l imaginary frequency

H = -3546.184309

G = -3546.318283

E(M06-2X-DCM) = -3546.658903

O	4.81556200	0.42602600	-1.43907100
O	5.01528000	-1.79381600	-0.14931600
P	4.17682100	-0.43099500	-0.23373500
O	4.40429100	0.41692200	1.02023300
N	2.61607200	-0.76563700	-0.47822800
S	1.98319600	-1.98935000	-1.29600500
C	1.69991300	-3.30693600	0.00343400
F	1.28087000	-4.42621300	-0.58380500
F	2.82180800	-3.55573400	0.68375000
F	0.75847700	-2.89263400	0.87016900

C	2.17913400	3.90536300	0.07710000
C	1.42699000	3.56053800	1.41277500
H	1.73853900	4.32890300	2.13546800
H	0.36986200	3.71529600	1.19907100
C	0.46720400	1.37661800	2.39002200
C	-0.83114100	1.91459800	2.52948600
C	0.63722800	-0.01351200	2.58765400
C	-1.90639200	1.09894000	2.87152500
H	-1.00366900	2.97572300	2.39944900
C	-0.44471900	-0.82580000	2.89931900
H	1.61201900	-0.46289500	2.43423800
C	-1.72155400	-0.27289800	3.04725800
H	-2.89434300	1.53580800	2.98000900
H	-0.29872900	-1.89556300	3.00689400
H	-2.56775900	-0.91681200	3.26622100
C	1.62360500	2.23366200	2.10749200
C	1.73734300	2.97657500	-1.12228800
H	2.63642200	2.53724800	-1.56706700
H	1.25405000	3.59344100	-1.88380100
N	0.84928200	1.85733800	-0.83653200
C	-0.51119400	1.89687900	-0.96171200
N	-1.06381700	0.64370200	-1.00622700
C	-2.38463600	0.20257500	-0.79996500
C	-3.53597200	0.95460300	-1.07130100
C	-2.52467700	-1.10709000	-0.30995500
C	-4.79400600	0.40540900	-0.81410800
C	-3.78775500	-1.63391200	-0.05799100
H	-1.64053000	-1.70522900	-0.11717800
C	-4.93792000	-0.88243700	-0.30229100
H	-5.92028000	-1.29732600	-0.11310000
C	-3.89894900	-2.99100200	0.58101900
C	-6.01904800	1.25128400	-1.04948200
F	-2.91962500	-3.82674200	0.17881100
F	-5.08108800	-3.58426400	0.31729600
F	-3.80083100	-2.90426200	1.93729100
F	-7.11106000	0.49486400	-1.30110200
F	-5.85978200	2.09502700	-2.08983600
F	-6.31009100	2.01095200	0.03362200
S	-1.36437600	3.35428600	-1.02856400
C	1.77438800	5.35994200	-0.25652600
H	2.10614700	6.05186500	0.52706100
H	2.24460600	5.67555700	-1.19526300
H	0.69088300	5.44995500	-0.37525800
C	3.71504000	3.86858400	0.20636200

H	4.16563500	4.26688900	-0.71079600
H	4.06048700	4.49954800	1.03463200
H	4.11378600	2.86128300	0.34467500
H	-3.44531000	1.95031700	-1.47996300
C	2.89497100	1.85187500	2.56094200
H	-0.40301300	-0.12929600	-1.11583800
H	3.64663300	2.63668700	2.62036400
H	2.93181100	1.14397200	3.38828900
O	2.86419100	-2.60483100	-2.29236500
H	1.29896200	0.94377500	-0.76242700
O	0.61529600	-1.60959200	-1.70077900
H	3.50283200	1.09663400	1.64016600
C	4.76876700	-0.04632300	-2.80461000
H	3.74279500	-0.02126800	-3.17998400
H	5.39514600	0.63975400	-3.37616700
H	5.15310900	-1.06601500	-2.87952000
C	6.40423900	-1.77109800	0.24155000
H	6.50435700	-1.36664700	1.25186000
H	6.73964400	-2.80820500	0.21400100
H	6.99150100	-1.17050300	-0.45964100

TS-1-3

l imaginary frequency

H = -3546.180537

G = -3546.315210

E(M06-2X-DCM) = -3546.652887

O	0.68417700	-2.41512800	-0.32409600
O	2.65785600	-2.49011200	-1.98232900
P	1.73802800	-1.48823300	-1.11861900
O	0.95445100	-0.51042900	-1.93491000
N	2.75323600	-0.76360700	-0.06307200
S	4.09843100	-1.13810300	0.59755500
C	5.48328500	-0.92913600	-0.65744400
F	5.30655300	0.20798100	-1.33676100
F	6.65162600	-0.88695900	-0.01916400
F	5.47700700	-1.95498100	-1.50533900
C	2.17530000	3.68675200	-0.38199000
C	1.70806600	3.62491800	1.13313000
H	2.31878500	4.35860300	1.67015400
H	0.68112800	3.99418300	1.15611500
C	0.63916600	1.53358700	2.26622800
C	-0.66781400	2.06240400	2.22996300
C	0.79642300	0.19001700	2.68472800
C	-1.76417700	1.28627200	2.59951700

H	-0.84807100	3.08222300	1.91622800
C	-0.30013800	-0.58474500	3.03400900
H	1.78272400	-0.25770500	2.69188100
C	-1.58873100	-0.03943800	2.99442100
H	-2.75825400	1.71898300	2.55133300
H	-0.15655500	-1.62033900	3.32837300
H	-2.44616500	-0.65651200	3.24474300
C	1.81858700	2.34816500	1.94692500
C	0.97525700	3.51330800	-1.35016300
H	1.35803300	3.61966600	-2.37610400
H	0.24691300	4.31031300	-1.18702900
N	0.25844900	2.25703500	-1.24336800
C	-1.09227000	2.13647800	-1.10176200
N	-1.49933400	0.83172900	-1.25523200
C	-2.70254500	0.21208900	-0.87180600
C	-3.97336500	0.77807800	-1.04232600
C	-2.59413900	-1.07640700	-0.32688300
C	-5.10367900	0.06449300	-0.63792800
C	-3.73288600	-1.77100500	0.07308200
H	-1.61323300	-1.52405900	-0.20247700
C	-5.00058000	-1.20699600	-0.07367400
H	-5.88701600	-1.74998100	0.23084100
C	-3.57169900	-3.09351600	0.76923500
C	-6.46084300	0.70612500	-0.77179300
F	-2.50828200	-3.79181800	0.30304700
F	-4.66015100	-3.87820700	0.64041000
F	-3.36353800	-2.92956400	2.10419700
F	-7.44022200	-0.21707200	-0.90680300
F	-6.52820800	1.52878000	-1.83909300
F	-6.76884100	1.44665800	0.31848000
S	-2.11920600	3.43483700	-0.74930000
C	2.70177400	5.11978800	-0.61851200
H	3.61519700	5.30103800	-0.04067400
H	2.94086600	5.27579500	-1.67679700
H	1.96009800	5.87350400	-0.32835700
C	3.28861100	2.68555000	-0.71962600
H	3.61717000	2.83433000	-1.75542000
H	4.16718800	2.82394900	-0.07960900
H	2.96185600	1.64778600	-0.61889400
H	-4.07208200	1.75828700	-1.48608400
C	3.06144800	2.00176800	2.47996700
H	-0.74104900	0.17150500	-1.45074600
H	3.86211300	2.73518400	2.40134000
H	3.06963200	1.43456300	3.41048600

O	4.28690500	-2.46840000	1.17710600
H	0.76056300	1.41064500	-1.51579800
O	4.44630900	0.01251900	1.56446600
H	3.64828600	0.92399500	1.78496500
C	1.09165300	-3.50537800	0.52549900
H	1.70437300	-3.14142500	1.35452800
H	0.16698700	-3.94809800	0.89720700
H	1.66089600	-4.24511500	-0.04466600
C	2.13013200	-3.06610600	-3.19620200
H	1.77743600	-2.27831600	-3.86617100
H	2.95558600	-3.61234000	-3.65410000
H	1.31003200	-3.75436100	-2.96859300

TS-2-1

l imaginary frequency

H = -3546.167524

G = -3546.301052

E(M06-2X-DCM) = -3546.644529

O	3.81947900	-1.72206300	2.31182900
P	3.62758900	-0.79839700	1.00990700
N	3.87840000	-1.77444900	-0.26422800
S	2.76669700	-2.41004800	-1.16789800
C	2.50627900	-1.15438300	-2.52977400
F	1.59636600	-1.60869300	-3.40956200
F	2.03790900	0.00376100	-2.01813800
F	3.64270900	-0.89781800	-3.17896500
C	-1.58174000	-4.03766100	0.88608000
C	-1.65790600	-3.48547700	-0.60106700
H	-0.63657400	-3.47520900	-0.98289400
H	-2.19026400	-4.25208900	-1.18121200
C	-3.70763300	-1.89831000	-0.84734700
C	-4.63290300	-2.96380000	-0.83612200
C	-4.22360100	-0.58307200	-0.81751600
C	-6.00387300	-2.72402100	-0.78654300
H	-4.28356600	-3.98625300	-0.90620400
C	-5.58904400	-0.34442700	-0.74384900
H	-3.54789000	0.26258400	-0.83177000
C	-6.48723300	-1.41625300	-0.72822600
H	-6.69491800	-3.56174500	-0.79553100
H	-5.95023400	0.67860700	-0.69801100
H	-7.55635400	-1.23125900	-0.67714200
C	-2.26339200	-2.14335800	-0.96793500
C	-1.34832800	-2.93385900	1.96010800
H	-0.86246500	-3.38760100	2.83295200

H	-2.29704300	-2.51585800	2.30404400
N	-0.56369600	-1.81473500	1.46431700
C	-0.92453400	-0.52911700	1.60482000
N	-0.27978000	0.23661300	0.54437900
C	-0.44535200	1.66158600	0.40423900
C	0.70011700	2.45134900	0.28576300
C	-1.71084300	2.23446800	0.27617300
C	0.56809700	3.81716300	0.03652400
C	-1.82623700	3.60158700	0.02750000
H	-2.59907800	1.63044400	0.38712800
C	-0.69132900	4.40274500	-0.09491000
H	-0.78684400	5.46400600	-0.29304200
C	-3.20111000	4.21016200	-0.06935100
C	1.80377100	4.65771500	-0.16326900
F	-4.09491300	3.32873300	-0.58557700
F	-3.20982600	5.30433700	-0.85812300
F	-3.67306800	4.58366400	1.13785300
F	2.87518100	4.13815900	0.47548400
F	1.62702900	5.91664800	0.29039300
F	2.12915500	4.75102100	-1.47222200
S	-2.03425500	0.08466600	2.67520400
C	-2.84944700	-4.80043200	1.31756400
H	-3.04802400	-5.64482500	0.64656400
H	-2.71330200	-5.21186000	2.32486900
H	-3.73517300	-4.15929200	1.34315000
C	-0.39845300	-5.03345200	0.88743600
H	-0.31768400	-5.52695100	1.86278000
H	-0.54667000	-5.81329000	0.13116800
H	0.55129100	-4.53707400	0.66732400
H	1.67557900	1.99288200	0.40322800
C	-1.41978800	-1.16385400	-1.52206800
H	-0.85193800	-0.43706900	-0.52846700
H	-0.46931000	-1.52135600	-1.91713500
H	-1.88527700	-0.37534100	-2.11242700
O	1.39902000	-2.46809500	-0.55582400
H	0.23169700	-2.03185000	0.85196900
O	3.21915000	-3.61304300	-1.86208500
O	4.94330800	0.13085800	1.10199900
C	3.72111300	-1.12277300	3.61496900
H	2.78835000	-0.55892600	3.71301800
H	3.73491200	-1.94566500	4.33194000
H	4.57500300	-0.46244700	3.79423000
C	5.19265200	1.09229400	0.06549200
H	6.20296800	1.47012300	0.23247500

H	5.13845100	0.61793600	-0.91997200
H	4.47812400	1.92010200	0.12515300
O	2.35880300	0.02200700	1.06608200
H	0.75021500	0.00481400	0.53659800

TS-2-1-1

l imaginary frequency

H = -3546.162530

G = -3546.296049

E(M06-2X-DCM) = -3546.631341

O	2.84351800	1.30325000	-1.12967300
O	3.06158600	1.75377800	1.29955400
P	2.52740700	2.43626000	-0.05319400
O	2.95112500	3.83158600	-0.27688800
N	0.81575200	2.23105900	-0.06271000
S	-0.26859500	3.33453900	0.50259800
C	-0.63298900	4.42085800	-0.98080800
F	-1.55952400	5.31075100	-0.61904900
F	0.45810700	5.04365400	-1.39550600
F	-1.11934300	3.65188900	-1.96005500
C	-4.72214200	0.75889400	-0.40753500
C	-4.22841800	0.46738900	1.07528100
H	-3.70762200	1.35751800	1.43411700
H	-5.12575800	0.37134800	1.70304500
C	-3.81138900	-2.08390500	1.20684000
C	-5.18398100	-2.39710500	1.32438100
C	-2.90204500	-3.14823500	1.00485900
C	-5.62581500	-3.71411600	1.24781700
H	-5.90388200	-1.61257700	1.52492100
C	-3.35124600	-4.45804400	0.89900100
H	-1.84668200	-2.93899700	0.87593400
C	-4.71315000	-4.74734900	1.02486000
H	-6.68309900	-3.93413700	1.36328500
H	-2.63849000	-5.25478000	0.70989600
H	-5.06075000	-5.77388700	0.95060900
C	-3.32806900	-0.71214100	1.36221400
C	-3.75758200	0.15138900	-1.46041000
H	-3.88822200	0.68169500	-2.41457300
H	-3.98552700	-0.89990200	-1.65395600
N	-2.38626700	0.20727700	-1.00704400
C	-1.40953000	-0.73409100	-1.22626000
N	-0.38126400	-0.50178900	-0.34523300
C	0.79209100	-1.26568700	-0.24404300
C	1.40414800	-1.98047000	-1.29203800

C	1.46219800	-1.21146400	0.99451700
C	2.62480800	-2.62352700	-1.08219000
C	2.67890500	-1.85812300	1.18642400
H	1.03053400	-0.63673200	1.80589800
C	3.27190200	-2.58371700	0.15218000
H	4.21384000	-3.09765800	0.30286000
C	3.41821600	-1.69725100	2.48557600
C	3.30569000	-3.28944600	-2.24822800
F	4.36962000	-0.72989200	2.39973000
F	4.05797400	-2.83154600	2.84608800
F	2.60221500	-1.34909800	3.50519900
F	2.43033800	-3.81828100	-3.12351600
F	4.13920500	-4.27720400	-1.85325700
F	4.06504400	-2.39812700	-2.94469800
S	-1.64307100	-2.00215800	-2.32156000
C	-6.13170400	0.20485700	-0.68969400
H	-6.87050300	0.63419600	-0.00204500
H	-6.44108900	0.46863800	-1.70788900
H	-6.17254700	-0.88473500	-0.60920000
C	-4.77957800	2.29708100	-0.55273300
H	-5.19057900	2.57204100	-1.53080900
H	-5.42750000	2.73607400	0.21557400
H	-3.79212900	2.75903700	-0.45501400
H	0.92639900	-2.02673100	-2.25976600
C	-2.02172400	-0.49408700	1.90343700
H	-1.21167000	-0.50838300	0.96688600
H	-1.85991800	0.50754600	2.30486300
H	-1.65401100	-1.28351900	2.56122800
O	0.30537100	4.18425100	1.53528400
H	-2.09169900	1.03911100	-0.50091700
O	-1.52440400	2.60080400	0.73212400
H	0.39783500	1.28758100	-0.22510700
C	4.19562300	0.80668600	-1.28449200
H	4.13491600	-0.00037000	-2.01322300
H	4.84509000	1.60497000	-1.65416700
H	4.56229600	0.42179800	-0.33026600
C	3.34919700	2.55472900	2.46729400
H	2.42159500	2.94736100	2.89309400
H	3.83387100	1.87591200	3.16928900
H	4.01249600	3.38232100	2.20650800

TS-2-1-2

l imaginary frequency

H = -3546.155757

G = -3546.289653

E(M06-2X-DCM) = -3546.628855

O	1.09190900	-2.50339400	1.62191700
P	2.16772800	-1.31363300	1.44779800
O	1.76978100	-0.02543000	2.13483900
N	2.25427200	-1.29077400	-0.18065800
S	3.39541500	-0.61586500	-1.02776100
C	4.36765500	-2.05464700	-1.71199800
F	4.87932400	-2.77241300	-0.70429000
F	3.58565700	-2.84259200	-2.45427500
F	5.37160500	-1.60043500	-2.47234500
C	2.04271300	3.61347200	0.63027600
C	0.88883100	3.83728200	1.70481800
H	1.11958000	3.22091700	2.57644200
H	0.95569600	4.88047100	2.04624200
C	-1.22220300	4.36475600	0.31734800
C	-0.83642900	5.69652800	0.04843600
C	-2.32300600	3.83395200	-0.39360700
C	-1.52552200	6.46295600	-0.88602500
H	-0.02545500	6.14924700	0.60599500
C	-2.98621100	4.59129900	-1.35115200
H	-2.62662800	2.80772000	-0.22238700
C	-2.59388500	5.91051400	-1.59614700
H	-1.22795500	7.49250200	-1.06101000
H	-3.81067400	4.15437600	-1.90622700
H	-3.12157200	6.50627900	-2.33532100
C	-0.54660200	3.56641600	1.34146600
C	1.59412200	2.61888700	-0.47079000
H	2.47949200	2.19160300	-0.95386400
H	1.00940600	3.12866300	-1.24257100
N	0.75433000	1.58656800	0.11368900
C	-0.24438700	0.88903200	-0.48262700
N	-1.15777100	0.44001000	0.33647200
C	-2.09992800	-0.56700000	0.07928900
C	-1.67133800	-1.88839800	-0.12729100
C	-3.47070400	-0.29147500	0.14886900
C	-2.61415600	-2.90539700	-0.26173800
C	-4.40147100	-1.32031900	-0.00008300
H	-3.81218200	0.72511900	0.31274400
C	-3.98257300	-2.63434000	-0.20360800
H	-4.70644400	-3.43154100	-0.31836300
C	-5.86872300	-1.00876800	0.12757400
C	-2.13043900	-4.32858900	-0.38238500
F	-6.63441100	-1.88908500	-0.54909100

F	-6.15984900	0.22883600	-0.33930500
F	-6.27459100	-1.04056900	1.41874200
F	-3.08856200	-5.14757200	-0.86997200
F	-1.77047900	-4.82227100	0.82958800
F	-1.05597700	-4.42991400	-1.18477100
S	-0.32348100	0.71457600	-2.25305000
C	2.48746800	4.91628100	-0.05917200
H	2.83858500	5.65098600	0.67537300
H	3.32272400	4.70881500	-0.73746800
H	1.69009600	5.37198100	-0.65379200
C	3.24836500	3.04376000	1.41172900
H	4.09800600	2.88536400	0.74061900
H	3.55599900	3.74353900	2.19893300
H	3.01377200	2.08125000	1.87613500
H	-0.60956500	-2.10921800	-0.15188400
C	-1.30376000	2.58927900	2.06453700
H	-1.33393500	1.57140300	1.37097200
H	-0.82914700	2.22987600	2.97929700
H	-2.36056700	2.82882700	2.19687700
O	4.38789400	0.17895200	-0.27153300
H	1.09234800	1.12297100	0.98336500
O	2.83445800	0.02780400	-2.24487100
H	1.02182200	0.48539100	-2.38736000
O	3.47490600	-1.96526100	2.14347400
C	0.64518800	-2.87413400	2.93264700
H	0.28890700	-1.99883000	3.48585100
H	-0.17478500	-3.57818100	2.78014600
H	1.45502800	-3.35852700	3.48729600
C	4.49333900	-1.14180800	2.74024000
H	5.14410800	-1.82211100	3.29388400
H	5.06099900	-0.62451900	1.96366000
H	4.04553600	-0.41431500	3.42313000

TS-2-1-3

l imaginary frequency

H = -3546.162530

G = -3546.296049

E(M06-2X-DCM) = -3546.631341

O	2.84351400	1.30325800	-1.12966900
O	3.06158000	1.75378100	1.29955900
P	2.52740000	2.43626500	-0.05318900
O	2.95111500	3.83159200	-0.27688000
N	0.81574500	2.23106000	-0.06270500
S	-0.26860400	3.33453900	0.50259900

C	-0.63299900	4.42085400	-0.98080900
F	-1.55953200	5.31075000	-0.61905200
F	0.45809700	5.04364700	-1.39551200
F	-1.11935700	3.65188300	-1.96005300
C	-4.72214100	0.75888500	-0.40754000
C	-4.22841700	0.46738400	1.07527600
H	-3.70762000	1.35751300	1.43411000
H	-5.12575700	0.37134400	1.70304000
C	-3.81138700	-2.08390900	1.20684100
C	-5.18397900	-2.39711000	1.32438300
C	-2.90204200	-3.14824000	1.00486100
C	-5.62581200	-3.71412100	1.24782300
H	-5.90388000	-1.61258100	1.52492300
C	-3.35124300	-4.45804900	0.89900600
H	-1.84668000	-2.93900100	0.87593500
C	-4.71314700	-4.74735400	1.02486700
H	-6.68309600	-3.93414300	1.36329200
H	-2.63848700	-5.25478500	0.70990300
H	-5.06074600	-5.77389300	0.95061800
C	-3.32806700	-0.71214600	1.36221200
C	-3.75757800	0.15138000	-1.46041500
H	-3.88822000	0.68168500	-2.41457800
H	-3.98552100	-0.89991100	-1.65396000
N	-2.38626300	0.20727200	-1.00704800
C	-1.40952500	-0.73409400	-1.22626100
N	-0.38125800	-0.50178600	-0.34523600
C	0.79209700	-1.26568400	-0.24404500
C	1.40415600	-1.98046500	-1.29204100
C	1.46220300	-1.21146100	0.99451600
C	2.62481600	-2.62352100	-1.08219300
C	2.67891100	-1.85811800	1.18642200
H	1.03053800	-0.63673000	1.80589600
C	3.27190900	-2.58371100	0.15217800
H	4.21384800	-3.09765200	0.30285800
C	3.41822100	-1.69724700	2.48557500
C	3.30569900	-3.28943800	-2.24823100
F	4.36962300	-0.72988600	2.39973100
F	4.05798100	-2.83154200	2.84608500
F	2.60221800	-1.34909700	3.50519800
F	2.43034900	-3.81826800	-3.12352300
F	4.13921100	-4.27719800	-1.85326100
F	4.06505800	-2.39811800	-2.94469600
S	-1.64306400	-2.00216600	-2.32155500
C	-6.13170100	0.20484300	-0.68970000

H	-6.87050100	0.63418300	-0.00205200
H	-6.44108600	0.46862200	-1.70789600
H	-6.17254200	-0.88474900	-0.60920300
C	-4.77958000	2.29707100	-0.55274100
H	-5.19058200	2.57202900	-1.53081800
H	-5.42750200	2.73606400	0.21556600
H	-3.79213200	2.75902900	-0.45502300
H	0.92640700	-2.02672500	-2.25976900
C	-2.02172200	-0.49408900	1.90343500
H	-1.21166800	-0.50838200	0.96688500
H	-1.85991900	0.50754300	2.30486300
H	-1.65400900	-1.28352100	2.56122600
O	0.30535800	4.18425400	1.53528400
H	-2.09169800	1.03910800	-0.50092300
O	-1.52441200	2.60080200	0.73212500
H	0.39783000	1.28758100	-0.22510300
C	4.19562000	0.80669800	-1.28448900
H	4.13491600	-0.00035700	-2.01322200
H	4.84508400	1.60498500	-1.65416300
H	4.56229400	0.42180900	-0.33026400
C	3.34918700	2.55473100	2.46730000
H	2.42158300	2.94735800	2.89310100
H	3.83386300	1.87591400	3.16929400
H	4.01248200	3.38232600	2.20651700

TS-2-1-4

l imaginary frequency

H = -3546.160293

G = -3546.294389

E(M06-2X-DCM) = -3546.631513

O	0.12790500	4.24676900	1.68047600
O	-0.83693100	4.35347300	-0.70022400
P	-0.00227300	3.43503800	0.30999400
O	1.34275600	2.97839900	-0.13240800
N	-1.03938700	2.11308700	0.49090400
S	-2.71182100	2.03928600	0.45481100
C	-3.11947600	1.94720000	-1.38829400
F	-4.28959900	1.33117400	-1.51584900
F	-3.19826200	3.17030100	-1.90547200
F	-2.17270700	1.25718800	-2.03091900
C	4.68524500	1.32044300	0.56561400
C	4.15472400	1.13046200	-0.91799700
H	3.52896500	1.99292900	-1.15585900
H	5.02624000	1.19181500	-1.58585300

C	3.97789800	-1.42556300	-1.30257000
C	5.36702500	-1.58958000	-1.49977800
C	3.18146700	-2.58830200	-1.18447500
C	5.93279200	-2.85807400	-1.57909000
H	6.00076500	-0.72176700	-1.63893000
C	3.75543600	-3.85220600	-1.23427400
H	2.11755100	-2.49814800	-0.99951300
C	5.13131600	-3.99289500	-1.43632100
H	6.99997200	-2.96099000	-1.75311300
H	3.12881200	-4.72956800	-1.10720300
H	5.57626600	-4.98284600	-1.48349400
C	3.36138500	-0.09863800	-1.29563900
C	3.79937000	0.55539700	1.58752400
H	3.88325800	1.04241300	2.56967000
H	4.14020600	-0.47447400	1.72010000
N	2.42362500	0.48492700	1.14929500
C	1.57210500	-0.57990600	1.32080200
N	0.48290800	-0.41356100	0.49946300
C	-0.55813700	-1.35763700	0.38454300
C	-1.11843000	-2.06301700	1.46706900
C	-1.15397200	-1.50306200	-0.87761300
C	-2.22361900	-2.88721000	1.26804000
C	-2.26691700	-2.32396700	-1.05962700
H	-0.75367600	-0.95512100	-1.72287400
C	-2.81136300	-3.02976500	0.00915700
H	-3.67832500	-3.66370000	-0.12902000
C	-2.91553200	-2.36393400	-2.41480400
C	-2.77081900	-3.67983700	2.42652200
F	-3.72865900	-3.43006900	-2.56602900
F	-1.99635200	-2.41097100	-3.41029300
F	-3.66609300	-1.25697500	-2.64194000
F	-4.10238000	-3.88946300	2.30583600
F	-2.56332100	-3.06369700	3.60890100
F	-2.19209100	-4.90142800	2.51076700
S	1.98607100	-1.90123400	2.29432000
C	6.13718700	0.84156400	0.75575100
H	6.82253900	1.37958200	0.08916000
H	6.46274600	1.03629900	1.78456700
H	6.24764400	-0.23134200	0.57733300
C	4.64542300	2.84049500	0.84369200
H	5.05905200	3.05777000	1.83533200
H	5.24900900	3.38459800	0.10637500
H	3.62557100	3.23433300	0.79823200
H	-0.69866500	-1.95159500	2.45603100

C	2.02114600	0.04040500	-1.78044900
H	1.25282700	-0.18682000	-0.84018300
H	1.73985600	1.06073800	-2.04599800
H	1.72276700	-0.69624800	-2.52866500
O	-3.26195500	3.30312500	0.93014000
H	2.02041600	1.32597000	0.73293900
O	-3.09476400	0.75211900	1.01287100
H	-0.54426500	1.18632000	0.51463600
C	-0.98353600	4.66540600	2.50468200
H	-1.46090100	3.79513700	2.95922600
H	-0.54980000	5.30291000	3.27587400
H	-1.72018400	5.21802000	1.91846100
C	-0.31147500	5.62923700	-1.12405700
H	0.62978900	5.48799700	-1.66195300
H	-1.06323800	6.05632300	-1.78774300
H	-0.15548000	6.28616400	-0.26346900

TS-2-1-5

l imaginary frequency

H = -3546.157571

G = -3546.290486

E(M06-2X-DCM) = -3546.630809

O	4.15175600	-1.71765400	-1.82710200
P	2.69580500	-1.87694400	-1.20398000
N	2.53140000	-0.80913800	-0.04208500
S	2.55986700	-0.96254100	1.54598500
C	4.38038200	-0.91910000	1.96694900
F	4.54007500	-1.04352600	3.28547200
F	5.01030300	-1.92762500	1.35052600
F	4.92171400	0.23728000	1.56807300
C	2.07140400	3.82013500	0.20767900
C	0.91109600	4.13572600	1.24215400
H	1.16937600	3.66949000	2.19675000
H	0.90632400	5.21793000	1.43457600
C	-1.22687100	4.33352700	-0.20528700
C	-0.91257800	5.63471900	-0.65077100
C	-2.30851700	3.66482500	-0.81945800
C	-1.64876900	6.24061600	-1.66492500
H	-0.11885000	6.19582900	-0.17222800
C	-3.02124400	4.26134700	-1.85365100
H	-2.56490300	2.65753200	-0.51374500
C	-2.69795400	5.55246900	-2.27742500
H	-1.40265700	7.25167400	-1.97643300
H	-3.82892000	3.71486700	-2.33089400

H	-3.26297700	6.02100900	-3.07826200
C	-0.50418500	3.71214300	0.91594100
C	1.63220700	2.67923200	-0.75127500
H	2.51464900	2.13636700	-1.11401400
H	1.10444500	3.06686600	-1.62591800
N	0.72545200	1.79748400	-0.05025200
C	-0.23992500	0.98057100	-0.60652800
N	-1.05009500	0.54560300	0.35848500
C	-2.04378300	-0.42354000	0.23127600
C	-1.82863300	-1.63403400	-0.45068700
C	-3.26529000	-0.24632300	0.90059300
C	-2.80673500	-2.62486500	-0.45397000
C	-4.24262200	-1.24104600	0.87557000
H	-3.45251300	0.67602300	1.43930000
C	-4.02589200	-2.44169700	0.20100600
H	-4.78728200	-3.21123800	0.18101800
C	-5.52091400	-1.03380500	1.64316800
C	-2.49813400	-3.94098300	-1.11491200
F	-6.54264000	-1.75090100	1.12739400
F	-5.89945200	0.26612700	1.64751600
F	-5.39323200	-1.40481800	2.93841400
F	-3.61146500	-4.63021400	-1.43603500
F	-1.75870400	-4.74243700	-0.30185900
F	-1.77393100	-3.78422100	-2.24823700
S	-0.34372400	0.73822800	-2.31085500
C	2.47772400	5.04104000	-0.63859100
H	2.82130200	5.86628200	-0.00302000
H	3.30754500	4.77462000	-1.30383600
H	1.65989000	5.40335800	-1.26735400
C	3.30060000	3.38482500	1.03707400
H	4.16289100	3.21362800	0.38271400
H	3.57769700	4.16667100	1.75501300
H	3.11608000	2.46181200	1.59506300
H	-0.89540300	-1.79095000	-0.97361700
C	-1.24150000	2.86454400	1.80283400
H	-1.25840800	1.73503500	1.24902700
H	-0.75860500	2.66003400	2.76024800
H	-2.30041900	3.10862900	1.90285400
O	2.07603300	-2.25264200	2.04787500
H	1.06487500	1.43376400	0.84411700
O	2.02511100	0.27799800	2.14012400
O	2.63245600	-3.42788700	-0.85989000
C	4.54448800	-2.47431000	-2.99397300
H	3.85210800	-2.28511900	-3.81869400

H	5.54255400	-2.12108900	-3.25419900
H	4.57203500	-3.54072500	-2.75724500
C	1.38487600	-4.10812600	-0.55155700
H	1.65420500	-5.15481500	-0.41042900
H	0.96335200	-3.70576400	0.37042400
H	0.69077700	-4.00705700	-1.38703600
O	1.62596700	-1.64284800	-2.34094100
H	1.06819100	-0.78920000	-2.29891200

TS-2-1-6

l imaginary frequency

H = -3546.158148

G = -3546.292272

E(M06-2X-DCM) = -3546.630499

O	-3.22095200	0.41112500	2.61532100
P	-3.28462400	-0.78964300	1.57731700
N	-4.24640400	-0.41817600	0.35935400
S	-3.86117000	0.48079100	-0.89680100
C	-3.42948800	-0.77852900	-2.21095200
F	-2.89624300	-0.14714900	-3.26485100
F	-2.52636800	-1.65299800	-1.73627300
F	-4.51256700	-1.44742400	-2.60078400
C	-0.64640600	4.34113100	0.17027900
C	-0.32984300	3.69828900	-1.25091300
H	-1.24611800	3.22135200	-1.60334500
H	-0.13973600	4.53362800	-1.93975400
C	2.18500200	3.06353100	-1.27231000
C	2.62419600	4.39341900	-1.45571900
C	3.16070600	2.08128000	-0.98430400
C	3.97306000	4.72060600	-1.35229200
H	1.91453500	5.16657300	-1.72550100
C	4.50240400	2.41358200	-0.85478200
H	2.85915300	1.05383200	-0.82254100
C	4.91450300	3.73672000	-1.04058900
H	4.29035200	5.74626000	-1.51662200
H	5.21867000	1.63713900	-0.60330000
H	5.96438200	3.99895400	-0.94547900
C	0.77996100	2.68739600	-1.43058300
C	-0.22201400	3.42845800	1.35547700
H	-0.82692100	3.68921700	2.23492700
H	0.82121300	3.59921100	1.63383500
N	-0.34169500	2.02300700	1.02715800
C	0.53435400	1.04223500	1.39525800
N	0.36460700	-0.04972200	0.55064000

C	1. 27556600	-1. 12661400	0. 41996500
C	2. 64311900	-1. 08467500	0. 73882900
C	0. 78099600	-2. 28118600	-0. 21724100
C	3. 47625000	-2. 15841900	0. 41960900
C	1. 62006100	-3. 35310600	-0. 50850600
H	-0. 26381000	-2. 32476500	-0. 50147200
C	2. 98108600	-3. 30355900	-0. 19803900
H	3. 63593100	-4. 13020100	-0. 44320700
C	1. 04075400	-4. 59857300	-1. 12624700
C	4. 94731100	-2. 00895000	0. 70398100
F	-0. 00478700	-4. 31996400	-1. 93617000
F	0. 58791000	-5. 45783400	-0. 18365000
F	1. 95646800	-5. 26819100	-1. 86039400
F	5. 18109300	-1. 64099800	1. 97977800
F	5. 49884400	-1. 04243500	-0. 08256000
F	5. 63652200	-3. 14429000	0. 47143700
S	1. 59362300	1. 24002800	2. 69470000
C	0. 04653800	5. 70217900	0. 37440000
H	-0. 25419100	6. 41808600	-0. 40013300
H	-0. 24255300	6. 12833700	1. 34245400
H	1. 13691500	5. 61877700	0. 36774100
C	-2. 17433000	4. 57459200	0. 19577600
H	-2. 46595500	5. 09072400	1. 11769400
H	-2. 48553600	5. 20103300	-0. 64879200
H	-2. 73151500	3. 63510000	0. 13380200
H	3. 04886500	-0. 22014900	1. 24620000
C	0. 45356400	1. 35948500	-1. 82635700
H	0. 37665400	0. 66340000	-0. 78076100
H	-0. 55342400	1. 22180600	-2. 22129000
H	1. 21980900	0. 82786200	-2. 39251400
O	-2. 58084700	1. 21828300	-0. 71879400
H	-1. 12076400	1. 74373100	0. 43169200
O	-5. 00926100	1. 21128400	-1. 41981100
O	-3. 96250500	-1. 97242700	2. 39499700
C	-2. 44879500	0. 31477600	3. 84077200
H	-1. 38527700	0. 20417100	3. 61638100
H	-2. 62177500	1. 25270600	4. 36807400
H	-2. 80665700	-0. 52489500	4. 44114500
C	-4. 27387800	-3. 22723200	1. 74938000
H	-4. 78733300	-3. 82892900	2. 49950100
H	-4. 92899400	-3. 05187000	0. 89251700
H	-3. 35334400	-3. 72604000	1. 43435800
O	-1. 83427800	-1. 30072600	1. 25639300
H	-1. 07115600	-0. 68906000	0. 88518400

TS-2-1-7

l imaginary frequency

H = -3546.149247

G = -3546.286009

E(M06-2X-DCM) = -3546.623723

O	-3.47688100	-0.89975800	1.99205300
P	-2.89450200	-2.13451600	1.17168000
N	-3.57733800	-2.28995300	-0.24667400
S	-3.41330000	-1.39750600	-1.56573400
C	-4.98502800	-0.38797600	-1.52334400
F	-5.00156300	0.44501800	-2.57319100
F	-6.06227800	-1.16982500	-1.57197000
F	-5.03201200	0.34732000	-0.39785800
C	-2.05058600	3.48446400	-0.48792200
C	-0.81104700	4.02983100	-1.31886600
H	-0.93316300	3.71256700	-2.35787400
H	-0.86852200	5.12689400	-1.34016900
C	1.15885100	4.14400600	0.35442900
C	0.67298100	5.31968300	0.96634700
C	2.25551400	3.48778600	0.95761300
C	1.25846800	5.81711300	2.12653000
H	-0.13675600	5.87531000	0.50938100
C	2.81894500	3.97182300	2.13246700
H	2.64126200	2.57110200	0.52809500
C	2.32635000	5.14000400	2.71918300
H	0.88148000	6.73545500	2.56723700
H	3.64183600	3.43326900	2.59221300
H	2.77489300	5.52251700	3.63162400
C	0.59200300	3.64552900	-0.90568600
C	-1.62057600	2.28666500	0.40194300
H	-2.49456500	1.66384500	0.63039300
H	-1.19144900	2.62176900	1.34906500
N	-0.60272400	1.52915300	-0.29243500
C	0.39192700	0.73994800	0.25316700
N	1.29475600	0.45964900	-0.68265900
C	2.37082800	-0.42223800	-0.53142100
C	2.19485500	-1.73418800	-0.05514200
C	3.64298600	-0.03373700	-0.97279400
C	3.27627700	-2.60906400	-0.00292300
C	4.71830300	-0.92185000	-0.91407700
H	3.79240500	0.96131800	-1.37743400
C	4.54842100	-2.21464400	-0.42564800
H	5.38001400	-2.90775700	-0.39535000

C	6.08300400	-0.44684200	-1.33442400
C	3.08399900	-3.99319500	0.56102500
F	6.88354400	-1.46624300	-1.70994200
F	6.71668200	0.20281100	-0.32813500
F	6.01553800	0.42125300	-2.37105300
F	3.92718300	-4.88592200	-0.00588000
F	1.82650100	-4.44781100	0.37409800
F	3.32077700	-4.02442100	1.89321800
S	0.40906300	0.34355500	1.93376400
C	-2.68780200	4.55786900	0.41393300
H	-3.03117600	5.41644700	-0.17549600
H	-3.56358000	4.14374400	0.92697200
H	-1.99871300	4.91776600	1.18332100
C	-3.11169200	3.03692800	-1.51765900
H	-4.02251600	2.70120900	-1.01324400
H	-3.37887400	3.86885400	-2.18054200
H	-2.76337300	2.20660000	-2.14039900
H	1.21121400	-2.06864900	0.24818700
C	1.45629200	2.95262000	-1.81193900
H	1.49098900	1.76345900	-1.40363000
H	1.07956300	2.85857900	-2.83216500
H	2.50427100	3.25458700	-1.77719000
O	-3.51370600	-2.21983900	-2.76714600
H	-0.86286100	1.21662300	-1.22395400
O	-2.34057300	-0.38454700	-1.47815000
O	-3.31409800	-3.39734500	2.04871600
C	-3.12970600	-0.66121500	3.37938800
H	-2.10924200	-0.27502200	3.44298300
H	-3.83706900	0.08923700	3.73365300
H	-3.23851700	-1.57979500	3.96036400
C	-3.00503900	-4.73401200	1.59026300
H	-3.43545700	-5.40945900	2.32998600
H	-3.45783700	-4.90329600	0.61056300
H	-1.92139000	-4.87256700	1.54087000
O	-1.31359000	-2.09247400	1.19674800
H	-0.84013400	-1.23535100	1.47322500

TS-E-1

l imaginary frequency

H = -3546.193030

G = -3546.327946

E(M06-2X-DCM) = -3546.664627

O	3.73926100	2.77126700	-0.72825000
O	4.52349800	1.39153900	1.29520800

P	3.28388200	1.58500800	0.27957300
O	3.08694000	0.27716500	-0.44329900
C	3.43103100	-3.22227800	-1.46941900
C	3.00446000	-3.34064500	0.03196900
H	3.66057200	-4.09560400	0.49501900
H	3.26144600	-2.40249700	0.52615500
C	0.96735200	-3.03281300	1.56273700
C	1.20633600	-1.66206600	1.81339900
C	0.04804300	-3.71203000	2.39646700
C	0.51631600	-0.98974100	2.81880300
H	1.88061900	-1.09395600	1.18142200
C	-0.61339800	-3.04489100	3.42097500
H	-0.11609300	-4.77682400	2.26461600
C	-0.39245400	-1.67930700	3.62504000
H	0.66853400	0.07740700	2.94436200
H	-1.30752100	-3.58709300	4.05621200
H	-0.93001600	-1.15302800	4.40850400
C	1.59838400	-3.72597500	0.43103100
C	2.33073300	-2.56249800	-2.36073800
H	1.68084200	-3.32128300	-2.79539100
H	2.83002500	-2.05271200	-3.19490600
N	1.47237200	-1.58860600	-1.68628600
C	0.13115600	-1.58656300	-1.68835000
N	-0.48354300	-0.46013300	-1.28309200
C	-1.85969500	-0.30520300	-0.94276200
C	-2.47902900	-1.13668000	-0.00825900
C	-2.55856400	0.76832100	-1.49844500
C	-3.81185400	-0.91385900	0.33480900
C	-3.88792500	0.98727700	-1.13761500
H	-2.06165600	1.42940300	-2.19857500
C	-4.52527200	0.14405000	-0.22803500
H	-5.55955400	0.31469400	0.04520500
C	-4.62842900	2.17552900	-1.69628500
C	-4.48683500	-1.85514400	1.29732600
F	-4.50330800	3.25949600	-0.90236300
F	-5.95153100	1.92268800	-1.81490500
F	-4.16849500	2.52089700	-2.91828500
F	-4.93087800	-2.97119600	0.67388000
F	-5.55260000	-1.28654500	1.89813600
F	-3.64041500	-2.26539400	2.27089900
S	-0.79017500	-2.98583700	-2.18146900
H	-1.92336900	-1.93994100	0.45837900
H	0.06915900	0.40500300	-1.15103700
H	1.96091300	-0.77076400	-1.27470300

C	0.87003100	-4.69073000	-0.26875200
H	1.39961900	-5.38129800	-0.91915400
H	0.17853900	-3.94328900	-1.17632300
H	-0.01649900	-5.11035000	0.20529900
N	2.09142500	2.18562800	1.19897900
S	0.64463300	2.53415500	0.66499000
O	-0.38945600	2.18994800	1.64783800
O	0.39713200	2.12675100	-0.75206900
C	0.61837000	4.39989200	0.57663800
F	0.84568500	4.91725900	1.78868800
F	-0.58091600	4.80891700	0.14844400
F	1.55578400	4.84329300	-0.26656000
C	4.71290900	-2.35734000	-1.48569200
H	5.48442700	-2.80184300	-0.84530500
H	5.12093000	-2.30214900	-2.50232900
H	4.51452700	-1.34229800	-1.13084700
C	3.78856000	-4.58320600	-2.10571600
H	4.13568000	-4.43785000	-3.13581100
H	4.60209000	-5.06588500	-1.55236800
H	2.94675200	-5.28057000	-2.14674500
C	4.63060900	2.47157500	-1.81099300
H	4.21341200	1.68643400	-2.44794900
H	4.74158500	3.39479600	-2.38293000
H	5.60976300	2.15404700	-1.43449700
C	4.88593000	2.45044400	2.19718300
H	4.05090900	2.68389900	2.86268400
H	5.73802300	2.08309800	2.77265400
H	5.17547300	3.34922400	1.64249600

NTPA-2R

0 imaginary frequency

H = -3240.820973

G = -3240.946808

E(M06-2X-DCM) = -3241.305406

O	1.21037900	1.07065800	-0.67193600
O	-1.08820400	0.82719700	0.50903700
P	-0.04573500	0.06172600	-0.47418200
O	-0.55896700	-0.41632200	-1.76512300
C	3.01636300	3.19881100	2.45361700
C	1.77378500	3.59270300	1.96865600
C	1.18152300	2.94250300	0.87188200
C	3.09088300	1.41466900	0.78986700
C	3.67855600	2.13617800	1.84070000
C	-1.84491900	1.83626700	-0.11886900

C	-1.27656900	3.09968000	-0.24651100
C	-1.91965100	4.05959700	-1.04223800
C	-3.16368000	3.79048400	-1.60338800
C	-3.76555000	2.55445800	-1.36251100
C	-3.11942800	1.54159100	-0.63371800
H	4.66362700	1.83623400	2.18589500
H	-4.75044800	2.34403800	-1.76861100
C	-0.05726400	3.71891300	0.42610900
C	-0.46047800	4.39471600	1.78089300
H	-1.08738900	5.27907400	1.63348700
H	-1.03356500	3.67455300	2.37595600
H	-1.00025400	5.66360000	-2.20045100
H	-1.46655500	6.12926600	-0.56845000
C	1.81344700	1.81504600	0.34805200
H	3.47194700	3.71483100	3.29479500
H	-3.66882500	4.53178800	-2.21743800
C	0.87939800	4.69994500	2.48036800
H	1.26725800	5.68727300	2.19333800
H	0.79771600	4.69975700	3.57313100
C	-1.06312400	5.30140800	-1.16810600
C	0.30254600	4.82465900	-0.62307300
H	0.90411300	5.63081700	-0.19168900
H	0.88489700	4.36784700	-1.43153000
C	-3.80908200	0.23411300	-0.40320000
C	-4.27952900	-0.08199700	0.89508500
C	-4.05904100	-0.63986500	-1.48812800
C	-4.09490500	0.77866300	2.02441100
C	-5.00665500	-1.31212300	1.10759300
C	-4.80876700	-1.85510800	-1.26316200
C	-4.56551200	0.44082700	3.26647800
H	-3.57658400	1.72124200	1.88721400
C	-5.47627000	-1.62983600	2.41991300
C	-5.25444900	-2.15959100	0.02499200
C	-5.26150000	-0.78350800	3.47351900
H	-4.40909700	1.11493400	4.10469600
H	-6.01271400	-2.56541100	2.56005500
H	-5.81149100	-3.07989300	0.18949000
H	-5.62314800	-1.03721100	4.46631600
C	3.82604200	0.26967800	0.16486800
C	4.33168300	0.39052400	-1.15302800
C	4.04756200	-0.91747000	0.90796000
C	4.18112600	1.57953100	-1.93581600
C	5.05202900	-0.71347500	-1.74499400
C	4.76691000	-2.01607200	0.29960100

C	4.68601100	1.66466500	-3.20674200
H	3.66233000	2.42872000	-1.50571900
C	5.55772100	-0.58565800	-3.07633900
C	5.24631400	-1.88344400	-1.00575000
C	5.37991300	0.56739500	-3.79119100
H	4.55742900	2.58003700	-3.77790800
H	6.09076000	-1.42983900	-3.50697800
H	5.78433300	-2.71350900	-1.45888400
H	5.76853200	0.65306900	-4.80208900
C	-3.87386100	-1.24277700	-3.84791200
H	-3.49892800	-1.02826800	-4.84505500
C	-3.59162700	-0.38477300	-2.81783600
H	-2.97910200	0.48985400	-2.99842100
C	-4.63561800	-2.42517800	-3.62565600
H	-4.84873700	-3.09279100	-4.45634300
C	-5.08105200	-2.72296300	-2.36666900
H	-5.65111400	-3.62983700	-2.17831900
C	3.76489600	-2.28305400	2.92060700
H	3.36817100	-2.40145100	3.92436500
C	4.48071300	-3.35455300	2.31804000
H	4.63143300	-4.27805500	2.86943800
C	4.96692900	-3.21886400	1.04560600
H	5.51151900	-4.03155400	0.57094000
C	3.56134800	-1.10599700	2.24563900
H	3.02064000	-0.29968000	2.72994100
N	0.58382000	-1.10403200	0.59789800
H	1.55680300	-1.04461600	0.89930200
S	-0.19264600	-2.50179000	1.10611800
C	0.41483700	-3.75970400	-0.14540500
O	-1.62178300	-2.34267700	0.90371700
O	0.40324400	-2.89350600	2.37626700
F	-0.03513600	-3.46345200	-1.35723000
F	1.75210800	-3.75882000	-0.14849200
F	-0.02712000	-4.96358500	0.22106600

NTPA-2R'

0 imaginary frequency

H = -3240.815105

G = -3240.939264

E(M06-2X-DCM) = -3241.302876

O	-1.23233500	1.07818800	0.59629600
O	1.03258900	0.78124700	-0.58712000
P	-0.07793700	0.00652000	0.28909200
C	-3.27061200	2.68509900	-2.69647800

C	-2.04084000	3.20527400	-2.30758100
C	-1.39708500	2.73063800	-1.15388200
C	-3.20834800	1.11768400	-0.81600100
C	-3.85629200	1.67716900	-1.93087600
C	1.67846200	1.90822000	-0.03492700
C	1.04522100	3.14643500	-0.08458800
C	1.62668100	4.22839900	0.59689800
C	2.86322700	4.09541700	1.21873100
C	3.52379000	2.86802700	1.16404900
C	2.94501600	1.74264400	0.55508300
H	-4.82936200	1.28342300	-2.20780700
H	4.50217900	2.75747800	1.62195400
C	-0.19757300	3.61653700	-0.83377000
C	0.15827900	4.12728500	-2.27091800
H	0.74112600	5.05321600	-2.25209900
H	0.75903600	3.36394800	-2.77856000
H	0.63049100	5.93639400	1.51694200
H	1.09635700	6.18945700	-0.16177100
C	-1.95189800	1.65007500	-0.47502100
H	-3.77665600	3.05955100	-3.58266600
H	3.31556300	4.93528200	1.73983600
C	-1.20634400	4.27418500	-2.97922000
H	-1.63463300	5.27383400	-2.82162800
H	-1.13631800	4.13003400	-4.06321500
C	0.71888400	5.43768300	0.54529200
C	-0.61621300	4.83103000	0.06327100
H	-1.25149800	5.54391600	-0.47084600
H	-1.18391500	4.45609300	0.92260100
C	3.69467800	0.44735300	0.52937200
C	4.24178400	-0.01768800	-0.69200700
C	3.92091900	-0.26566600	1.73214700
C	4.08268400	0.67891200	-1.93285800
C	5.01893600	-1.23595200	-0.70569200
C	4.70982700	-1.47717600	1.70324000
C	4.62581100	0.19941600	-3.09610800
H	3.52538400	1.60895200	-1.94564400
C	5.56405200	-1.70442800	-1.94169500
C	5.23124100	-1.92926500	0.48865200
C	5.37313400	-1.01228500	-3.10660100
H	4.48794500	0.74988000	-4.02293000
H	6.13885500	-2.62745800	-1.93212700
H	5.81971200	-2.84436600	0.47273600
H	5.79260700	-1.37865900	-4.03949400
C	-3.87182400	0.02399300	-0.04177000

C	-4.29397300	0.26270200	1.29035600
C	-4.14196400	-1.21849800	-0.66759800
C	-4.10369300	1.51398300	1.96068400
C	-4.97850700	-0.78244700	2.01667400
C	-4.85108200	-2.24313700	0.06500300
C	-4.52388400	1.70693900	3.25086600
H	-3.62552700	2.32867600	1.42837300
C	-5.39373000	-0.54322700	3.36395900
C	-5.23946400	-2.00097400	1.38454200
C	-5.17128600	0.66313200	3.97042000
H	-4.36544200	2.66883700	3.73142000
H	-5.89774200	-1.34713800	3.89533300
H	-5.76311000	-2.78084900	1.93380400
H	-5.49281500	0.83256000	4.99441600
C	3.63422100	-0.56554400	4.14122600
H	3.21445700	-0.22966500	5.08561600
C	3.39002900	0.14890800	2.99737900
H	2.77102000	1.03710900	3.04014800
C	4.42381200	-1.75026800	4.10811200
H	4.60452800	-2.30296900	5.02584800
C	4.94069000	-2.19137900	2.92063800
H	5.53684600	-3.09970200	2.87763400
C	-4.03371200	-2.73212900	-2.58229700
H	-3.70286500	-2.94067500	-3.59612100
C	-4.75495600	-3.72674600	-1.86411200
H	-4.97894200	-4.67799700	-2.33880900
C	-5.14253100	-3.48807900	-0.57464000
H	-5.67765700	-4.24447400	-0.00558700
C	-3.73287700	-1.52696100	-2.00520400
H	-3.15506900	-0.79725100	-2.55947600
N	-0.57154300	-1.24822400	-0.53737000
S	-0.25849800	-2.77435800	-0.13448000
C	1.10076100	-3.23109000	-1.32982900
O	-1.37189600	-3.66076200	-0.43766400
O	0.38726000	-2.86395600	1.20549400
F	2.13876300	-2.40471700	-1.16366000
F	1.49319600	-4.48428900	-1.09104600
F	0.66114900	-3.13903300	-2.58514800
O	0.48400100	-0.26789100	1.73797400
H	0.60562400	-1.25542700	1.85034100

NTPA-2R'-1

0 imaginary frequency

H = -3240.814424

G = -3240.937395

E(M06-2X-DCM) = -3241.302748

O	-0.89169200	1.11370100	0.64817700
O	1.32275300	0.77781800	-0.63292700
P	0.15775100	0.00168400	0.17090300
C	-2.71656300	3.53222500	-2.25187600
C	-1.42904500	3.81607000	-1.81040700
C	-0.84116700	3.06500800	-0.77920600
C	-2.84402500	1.65700500	-0.68360500
C	-3.42151900	2.48449800	-1.66252100
C	2.12454900	1.70213800	0.06720200
C	1.65143400	2.99452100	0.26105500
C	2.37799500	3.86233400	1.09219700
C	3.60474300	3.47513200	1.62074300
C	4.10458800	2.20591100	1.32502600
C	3.37197800	1.28138200	0.56300600
H	-4.43949600	2.27372300	-1.97494500
H	5.07202000	1.90056800	1.71237400
C	0.46286000	3.73130200	-0.34463100
C	0.86485600	4.44620800	-1.67894200
H	1.55913900	5.27561800	-1.51400200
H	1.36084900	3.71967100	-2.33261400
H	1.61227700	5.47781300	2.34176900
H	2.07106700	5.97731600	0.71748900
C	-1.52634500	1.95452600	-0.29068700
H	-3.17528000	4.12213100	-3.04124100
H	4.17273900	4.14933400	2.25669600
C	-0.47637200	4.88175500	-2.30534500
H	-0.77761200	5.87946000	-1.95686400
H	-0.43602500	4.93000200	-3.39929200
C	1.62103800	5.15720800	1.29400200
C	0.21182000	4.80568300	0.76773300
H	-0.34196800	5.67208200	0.39378300
H	-0.38035100	4.35157600	1.57057500
C	3.92339900	-0.08322500	0.29423500
C	4.32922100	-0.42761600	-1.01909600
C	4.08251500	-1.00645600	1.35727100
C	4.24008200	0.47725000	-2.12518200
C	4.88297700	-1.73787800	-1.27249700
C	4.65136900	-2.30836700	1.08888300
C	4.64159600	0.10952700	-3.38270100
H	3.85363300	1.47636700	-1.95723400
C	5.28316600	-2.08420500	-2.60067900
C	5.02836600	-2.63879100	-0.21465800

C	5.16473100	-1.19103400	-3.63031000
H	4.56171000	0.81793400	-4.20296500
H	5.68578300	-3.07948300	-2.77220700
H	5.44518100	-3.62418000	-0.41171000
H	5.47062700	-1.46645200	-4.63573100
C	-3.65789100	0.54898700	-0.09465700
C	-4.03353700	0.59761800	1.27184200
C	-4.14287100	-0.48657400	-0.93267700
C	-3.62632000	1.64417800	2.16065700
C	-4.89706500	-0.42979800	1.80858400
C	-5.04525500	-1.47743400	-0.39061500
C	-4.00513900	1.65384700	3.47762900
H	-3.01167100	2.45079400	1.77788500
C	-5.26245800	-0.38772900	3.19051200
C	-5.38481000	-1.42969500	0.96327900
C	-4.82712400	0.61961300	4.00769300
H	-3.67822800	2.46202700	4.12651400
H	-5.90344500	-1.17731700	3.57557200
H	-6.05415900	-2.18581800	1.36882500
H	-5.11257600	0.64100600	5.05583500
C	3.85707400	-1.64413800	3.70743400
H	3.54335500	-1.40223800	4.71945000
C	3.68593000	-0.72374700	2.70580900
H	3.22918700	0.23327000	2.92874200
C	4.43386400	-2.91798900	3.43887800
H	4.56012500	-3.63365700	4.24649200
C	4.81394300	-3.23707300	2.16389400
H	5.24385900	-4.21026900	1.93978700
C	-4.30022900	-1.60203500	-3.10215600
H	-3.99618400	-1.67727900	-4.14253300
C	-5.22536800	-2.54593600	-2.57307300
H	-5.63390800	-3.31936600	-3.21760700
C	-5.57531700	-2.48862600	-1.25182200
H	-6.26293100	-3.21607000	-0.82676600
C	-3.77497500	-0.61353400	-2.31171800
H	-3.05144800	0.07698100	-2.72821000
N	-0.45029400	-1.09650900	-0.79267100
S	-0.01789600	-2.64773100	-0.69902300
C	-1.58492900	-3.45073000	-0.07634300
O	0.95976900	-2.87532700	0.40121800
O	0.24394000	-3.23610700	-2.00527000
F	-1.31572100	-4.71756200	0.25154300
F	-2.02669100	-2.80326900	1.00846600
F	-2.52426800	-3.43217600	-1.01836900

O	0.71432400	-0.48241100	1.56956500
H	0.99860200	-1.43376700	1.47786000

NTPA-2R' -2

0 imaginary frequency

H = -3240.805121

G = -3240.929781

E(M06-2X-DCM) = -3241.298742

O	1.20409900	-0.92438500	0.36613900
O	-1.16837400	-0.34272100	-0.51888900
P	0.03615200	0.17973200	0.42123600
C	3.17036900	-1.15711000	-3.32047700
C	1.92918800	-1.76108400	-3.14950500
C	1.32086100	-1.79530200	-1.88545400
C	3.19747200	-0.52600900	-0.95672900
C	3.81251500	-0.59289400	-2.21795900
C	-1.70753300	-1.63194400	-0.37639300
C	-1.05598400	-2.70694700	-0.97010800
C	-1.55569700	-4.00006300	-0.74224800
C	-2.72066500	-4.19654900	-0.00810200
C	-3.39409400	-3.09117000	0.51378200
C	-2.89919400	-1.78773900	0.35498500
H	4.80355900	-0.16378700	-2.32931300
H	-4.31454600	-3.22956100	1.07344700
C	0.13743700	-2.76095500	-1.91949500
C	-0.28582600	-2.61973200	-3.41853500
H	-0.87213500	-3.47495500	-3.76942600
H	-0.90121500	-1.71977500	-3.52801800
H	-0.47584400	-5.89597400	-0.71570800
H	-1.08412100	-5.42759500	-2.30073000
C	1.91398800	-1.08812100	-0.84439700
H	3.64686100	-1.13532400	-4.29709500
H	-3.10581000	-5.19873900	0.16139800
C	1.04817200	-2.43655600	-4.17910200
H	1.46649800	-3.40196100	-4.49610200
H	0.93292800	-1.83065200	-5.08459100
C	-0.64989400	-5.03496900	-1.37064400
C	0.63326300	-4.22494100	-1.64687200
H	1.23044200	-4.62137900	-2.47303100
H	1.26501000	-4.22079600	-0.75109100
C	-3.64333500	-0.62132500	0.93029400
C	-4.39088000	0.22087500	0.07141900
C	-3.64007200	-0.39285600	2.32868500
C	-4.47993400	0.00450100	-1.34067400

C	-5.12026300	1.33879000	0.62559100
C	-4.38428000	0.72404500	2.87026000
C	-5.21385300	0.83735400	-2.14375500
H	-3.95508000	-0.83822300	-1.77643600
C	-5.86554000	2.18967100	-0.24895200
C	-5.09402700	1.56090800	2.00494300
C	-5.91275000	1.94998300	-1.59541600
H	-5.26279700	0.65058400	-3.21295800
H	-6.39964800	3.03166800	0.18453000
H	-5.64572500	2.40340800	2.41680900
H	-6.48371100	2.60245500	-2.25003200
C	3.92519200	0.06557200	0.20945000
C	4.32614000	-0.77753900	1.27759700
C	4.27549500	1.43826100	0.21273500
C	4.05489600	-2.18357700	1.31174200
C	5.07319900	-0.22010800	2.38229000
C	5.04029300	1.97518900	1.31677400
C	4.45814300	-2.96718100	2.36145800
H	3.52858400	-2.63751800	0.47963100
C	5.46862700	-1.07039600	3.46190700
C	5.41005800	1.13589400	2.36998300
C	5.16858100	-2.40548500	3.45953800
H	4.23829100	-4.03161300	2.35532300
H	6.02184300	-0.62732900	4.28682500
H	5.97868200	1.54789600	3.20147100
H	5.47672500	-3.04107100	4.28527600
C	-2.93592700	-0.96542600	4.60037900
H	-2.37656100	-1.60665000	5.27599200
C	-2.91760200	-1.21885600	3.25295600
H	-2.34083400	-2.05242500	2.86921100
C	-3.67613300	0.13157000	5.12720100
H	-3.67788300	0.31514900	6.19793600
C	-4.37589700	0.95040700	4.28276500
H	-4.94171600	1.79412600	4.67044600
C	4.24326700	3.66564800	-0.78884000
H	3.90871300	4.33153500	-1.57834000
C	5.01636300	4.18312300	0.28812200
H	5.28784800	5.23522400	0.29891800
C	5.39840900	3.35937900	1.31179700
H	5.97811600	3.74276300	2.14833400
C	3.88871200	2.34246700	-0.82789100
H	3.27824300	1.97854200	-1.64567000
N	0.32610700	1.68671500	0.12404800
S	0.28116700	2.56123000	-1.24339300

C	-1.56148200	2.77013000	-1.58462100
O	0.79790000	1.83087200	-2.40756600
O	0.75725300	3.90781200	-0.94589800
F	-2.01926400	1.74772200	-2.31064600
F	-2.25303800	2.83821100	-0.43949800
F	-1.74114900	3.90187600	-2.26892800
O	-0.34096000	-0.04751500	1.95103600
H	-0.98537000	0.60293500	2.28058400

NTPA-2R-1

0 imaginary frequency

H = -3240.813507

G = -3240.938401

E(M06-2X-DCM) = -3241.296948

O	0.95572800	-1.07033500	-0.09212600
O	-1.30912300	0.07386000	-0.55487500
P	-0.15668500	-0.08903300	0.55961100
O	-0.49425100	-0.51770600	1.92544100
C	3.15912200	0.41782600	-3.31270200
C	1.85343700	-0.02034100	-3.50655400
C	1.14993900	-0.65188700	-2.46775100
C	3.06460700	-0.31843300	-0.98341700
C	3.77050300	0.21603000	-2.07247500
C	-1.94082300	-1.04060700	-1.12614900
C	-1.34501000	-1.66500700	-2.21765700
C	-1.95197500	-2.81999000	-2.73822500
C	-3.15906400	-3.28551300	-2.22773400
C	-3.76452300	-2.59939700	-1.17512700
C	-3.16683700	-1.47173000	-0.59056200
H	4.80888400	0.49945500	-1.92726000
H	-4.71230200	-2.94545700	-0.77363700
C	-0.10806800	-1.30447300	-3.03633600
C	-0.41346100	-0.32371500	-4.21442400
H	-1.04957900	-0.77719200	-4.98116100
H	-0.92954100	0.55584600	-3.81623000
H	-1.03385500	-4.50888600	-3.77129300
H	-1.51280500	-3.18343400	-4.82818200
C	1.72055500	-0.68015400	-1.20017600
H	3.70939900	0.89650700	-4.11876300
H	-3.62632600	-4.17709800	-2.63810100
C	0.98309900	0.08543300	-4.74198100
H	1.32921700	-0.58892200	-5.53739500
H	0.98922500	1.09734900	-5.16209600
C	-1.10162900	-3.41714200	-3.83600800

C	0.25471200	-2.72030100	-3.61212300
H	0.86843700	-2.65733700	-4.51535600
H	0.82841900	-3.27007700	-2.85683000
C	-3.84246200	-0.77343500	0.54795100
C	-4.46784400	0.47763400	0.33052900
C	-3.90262200	-1.39532300	1.81770900
C	-4.46174100	1.14100800	-0.93824600
C	-5.16659700	1.12121800	1.41939800
C	-4.61782900	-0.74625800	2.89303600
C	-5.07801700	2.35225300	-1.11266300
H	-3.95840700	0.66987500	-1.77535500
C	-5.79556600	2.38543800	1.19492000
C	-5.22518600	0.49122400	2.66543600
C	-5.75256900	2.98863900	-0.03254200
H	-5.05211200	2.83547700	-2.08557600
H	-6.31159600	2.85734200	2.02784600
H	-5.75873600	0.97725200	3.47998700
H	-6.23218900	3.95090600	-0.18953100
C	3.73764300	-0.55071300	0.33444400
C	3.96854500	-1.88087000	0.77030600
C	4.18482100	0.53876800	1.12046300
C	3.59652100	-3.02972000	0.00075700
C	4.63145200	-2.11366100	2.03340100
C	4.85605600	0.29035700	2.37694300
C	3.83514500	-4.30161700	0.45166500
H	3.12529800	-2.88450600	-0.96458200
C	4.85462400	-3.45644000	2.47137400
C	5.05351000	-1.02516200	2.80139100
C	4.46622100	-4.52341900	1.70801100
H	3.54265000	-5.15315400	-0.15690300
H	5.34652200	-3.60860000	3.42915500
H	5.55235100	-1.20771700	3.75103800
H	4.64233700	-5.53911200	2.05134000
C	-3.36086800	-3.22713600	3.34087500
H	-2.86587800	-4.17579900	3.53016400
C	-3.27137900	-2.64911200	2.10207400
H	-2.70226400	-3.13904500	1.32032000
C	-4.08328900	-2.59250500	4.39099900
H	-4.14258500	-3.06687600	5.36685600
C	-4.68811700	-1.38510200	4.17040000
H	-5.23397200	-0.88353400	4.96617200
C	4.43211700	2.93877900	1.51526300
H	4.26364300	3.96310000	1.19502700
C	5.10132800	2.68806600	2.74688700

H	5.44573100	3.52143900	3.35306900
C	5.30222000	1.39956300	3.16206800
H	5.80683600	1.19212300	4.10275300
C	3.99017200	1.90293700	0.73379100
H	3.47901900	2.10844800	-0.19697100
N	0.43173300	1.53358800	0.49173100
H	0.63921300	1.86194700	1.43597400
S	-0.29529400	2.78542000	-0.41763600
C	1.02316600	4.10360100	-0.17713400
O	-1.47537100	3.31509200	0.25245100
O	-0.28694300	2.43165100	-1.82916800
F	0.48431900	5.27302300	-0.50877000
F	1.40335100	4.13581000	1.10749700
F	2.08269000	3.87285400	-0.95016900

NTPA-2R-2

0 imaginary frequency

H = -3240.820887

G = -3240.944275

E(M06-2X-DCM) = -3241.306621

O	-1.25957000	0.93502000	0.38373500
O	1.09126900	0.26184600	-0.44426100
P	-0.06474100	-0.13102000	0.61907600
O	0.25234200	-0.24156200	2.05094200
C	-3.19585200	1.04096600	-3.32270300
C	-1.94842200	1.63514300	-3.16853800
C	-1.34252600	1.71007900	-1.90450200
C	-3.22565600	0.48286400	-0.94287900
C	-3.84209500	0.51348300	-2.20380200
C	1.67684200	1.54100500	-0.37017100
C	1.05250000	2.60259900	-1.02009100
C	1.58137200	3.89409200	-0.85760200
C	2.74732900	4.10258400	-0.12965800
C	3.39154200	3.01014700	0.44984800
C	2.86994600	1.71010500	0.35709100
H	-4.83545500	0.08594700	-2.30296000
H	4.31115500	3.15494400	1.00903100
C	-0.13660200	2.64239600	-1.97668400
C	0.28781800	2.42139600	-3.46565500
H	0.90272500	3.24047900	-3.85196000
H	0.87292500	1.49722200	-3.53067800
H	0.55054600	5.81544000	-0.92719500
H	1.14677400	5.25414900	-2.48653000
C	-1.93997500	1.04740000	-0.83798100

H	-3.67066200	0.99170600	-4.29922100
H	3.15349200	5.10352600	-0.00824500
C	-1.04917400	2.24607000	-4.22247800
H	-1.43992700	3.20939000	-4.57857100
H	-0.95023900	1.60120200	-5.10265900
C	0.70305200	4.91895600	-1.53851500
C	-0.59866600	4.12843100	-1.77564400
H	-1.18751000	4.49862700	-2.61986500
H	-1.22925300	4.18144100	-0.88059200
C	3.61094200	0.57901500	1.00355600
C	4.42437900	-0.26195900	0.20700900
C	3.56759800	0.41249800	2.40774900
C	4.56737900	-0.09177000	-1.20737000
C	5.17613100	-1.32602200	0.83265900
C	4.33891200	-0.64497000	3.02200600
C	5.36828900	-0.92065300	-1.94922200
H	4.02938000	0.71403700	-1.69468800
C	5.99030300	-2.17600900	0.02069500
C	5.10900100	-1.49000400	2.21893500
C	6.08589900	-1.98407600	-1.33134000
H	5.45897500	-0.76658800	-3.02121100
H	6.54113400	-2.97747500	0.50750700
H	5.68201700	-2.28842300	2.68641600
H	6.71222800	-2.63417500	-1.93615100
C	-3.94140200	-0.09255400	0.23930300
C	-4.36380700	0.76637500	1.28564400
C	-4.24342200	-1.47590300	0.28933600
C	-4.14161700	2.18091000	1.27065600
C	-5.07649600	0.21709700	2.41653400
C	-4.96459200	-2.00911600	1.42435500
C	-4.56537700	2.98288200	2.29782700
H	-3.63534700	2.62322300	0.42022200
C	-5.49484900	1.08724700	3.47137900
C	-5.35432600	-1.15174500	2.45582100
C	-5.24591300	2.43167700	3.42008700
H	-4.38352500	4.05353600	2.25645900
H	-6.02189800	0.65189700	4.31711500
H	-5.89152700	-1.55939200	3.30988600
H	-5.57006300	3.08271800	4.22735100
C	2.78694100	1.07465000	4.62469100
H	2.18232900	1.72341500	5.25237100
C	2.78872100	1.25259900	3.26684600
H	2.18094700	2.03350400	2.82543800
C	3.55485600	0.03664800	5.22532200

H	3.53702800	-0.09000700	6.30442900
C	4.30301300	-0.80025000	4.44316100
H	4.88937400	-1.60093400	4.88785100
C	-4.14519900	-3.73247400	-0.64863600
H	-3.81322600	-4.40548400	-1.43342500
C	-4.86516900	-4.24852100	0.46594000
H	-5.09246600	-5.30988700	0.51567000
C	-5.26008900	-3.40771200	1.47103900
H	-5.80591700	-3.78811400	2.33133500
C	-3.84859000	-2.39686900	-0.73459900
H	-3.29905500	-2.02482300	-1.59114600
N	-0.48184800	-1.64467100	-0.05131300
H	-0.75969700	-2.33782500	0.64035500
S	-0.24708100	-2.35448400	-1.55958300
C	1.62942500	-2.54748100	-1.73331100
O	-0.65386200	-1.44675900	-2.62190300
O	-0.77115900	-3.70894100	-1.42460300
F	1.84603200	-3.67534600	-2.40968900
F	2.12517900	-1.52267400	-2.41532600
F	2.19830800	-2.62950700	-0.53363700

NTPA-2R-3

0 imaginary frequency

H = -3240.820890

G = -3240.944266

E(M06-2X-DCM) = -3241.306619

O	-1.25963700	0.93502400	0.38425400
O	1.09120100	0.26207600	-0.44387100
P	-0.06494600	-0.13141400	0.61908900
O	0.25185900	-0.24292700	2.05094900
C	-3.19585600	1.04284600	-3.32217200
C	-1.94843500	1.63698700	-3.16765900
C	-1.34257400	1.71123600	-1.90357400
C	-3.22566700	0.48343800	-0.94263300
C	-3.84208400	0.51472200	-2.20357100
C	1.67683200	1.54116900	-0.36927200
C	1.05253700	2.60311400	-1.01864800
C	1.58157700	3.89448900	-0.85563300
C	2.74768900	4.10253000	-0.12782800
C	3.39186600	3.00973900	0.45110000
C	2.87007200	1.70982600	0.35790400
H	-4.83542300	0.08718700	-2.30298200
H	4.31160500	3.15417400	1.01017800
C	-0.13661500	2.64354400	-1.97518900

C	0.28785000	2.42326700	-3.46430100
H	0.90287100	3.24248500	-3.85015100
H	0.87284400	1.49905300	-3.52974900
H	0.55080600	5.81586200	-0.92390500
H	1.14689300	5.25565400	-2.48368200
C	-1.94003300	1.04797900	-0.83740800
H	-3.67062200	0.99405200	-4.29873700
H	3.15399800	5.10336900	-0.00604400
C	-1.04915000	2.24850700	-4.22123300
H	-1.43981500	3.21213600	-4.57661600
H	-0.95031500	1.60427400	-5.10188500
C	0.70324400	4.91980200	-1.53587200
C	-0.59854200	4.12948100	-1.77338900
H	-1.18732200	4.50015200	-2.61745100
H	-1.22918000	4.18212000	-0.87835400
C	3.61091400	0.57836400	1.00390900
C	4.42438200	-0.26228900	0.20705000
C	3.56737100	0.41116200	2.40801000
C	4.56753200	-0.09141700	-1.20723300
C	5.17592000	-1.32676300	0.83225800
C	4.33845500	-0.64673700	3.02183600
C	5.36843300	-0.92002500	-1.94941400
H	4.02969000	0.71471300	-1.69419400
C	5.99009000	-2.17643400	0.01996000
C	5.10855000	-1.49146000	2.21844300
C	6.08585900	-1.98383600	-1.33197500
H	5.45928300	-0.76541700	-3.02131300
H	6.54077600	-2.97821400	0.50642400
H	5.68132300	-2.29025300	2.68559100
H	6.71216900	-2.63372100	-1.93704000
C	-3.94135200	-0.09271700	0.23921500
C	-4.36375300	0.76555900	1.28609900
C	-4.24320200	-1.47611700	0.28846700
C	-4.14180700	2.18013900	1.27186500
C	-5.07614400	0.21552200	2.41681300
C	-4.96411000	-2.01009900	1.42329700
C	-4.56554000	2.98146600	2.29955600
H	-3.63578800	2.62302300	0.42157200
C	-5.49443400	1.08500200	3.47223800
C	-5.35374800	-1.15339600	2.45536000
C	-5.24575500	2.42951100	3.42164900
H	-4.38391800	4.05218100	2.25872300
H	-6.02123900	0.64907300	4.31783000
H	-5.89066000	-1.56164600	3.30932000

H	-5.56984600	3.08004100	4.22935100
C	2.78660400	1.07236900	4.62520500
H	2.18209700	1.72098000	5.25314900
C	2.78856300	1.25098800	3.26744900
H	2.18104900	2.03228700	2.82636700
C	3.55423400	0.03389900	5.22540600
H	3.53622500	-0.09332000	6.30444600
C	4.30233500	-0.80274000	4.44291100
H	4.88850100	-1.60375300	4.88727000
C	-4.14497900	-3.73208800	-0.65095900
H	-3.81318100	-4.40456100	-1.43629000
C	-4.86466200	-4.24890500	0.46345300
H	-5.09184800	-5.31032500	0.51257400
C	-5.25944500	-3.40875900	1.46916900
H	-5.80505800	-3.78975600	2.32934200
C	-3.84849600	-2.39639900	-0.73613500
H	-3.29918500	-2.02374200	-1.59256800
N	-0.48222200	-1.64452800	-0.05240000
H	-0.76038600	-2.33817500	0.63865000
S	-0.24714600	-2.35338000	-1.56112300
C	1.62946500	-2.54598400	-1.73489100
O	-0.65396300	-1.44504600	-2.62289800
O	-0.77107100	-3.70798100	-1.42697300
F	1.84625000	-3.67345000	-2.41188600
F	2.12502100	-1.52070300	-2.41630700
F	2.19835700	-2.62863500	-0.53523700

NTPA-2R-anion-1

0 imaginary frequency

H = -3240.322970

G = -3240.447065

E(M06-2X-DCM) = -3240.862063

O	1.21076300	0.06398000	-0.55431800
O	-1.09368400	1.03480300	0.13621100
P	0.08144600	-0.02607000	0.67177900
O	0.58291300	0.50443500	1.95922000
C	2.88362500	3.78232100	-1.46135700
C	1.70137300	3.36289800	-2.06411000
C	1.17137800	2.09511000	-1.79104000
C	3.01135000	1.65549800	-0.25456800
C	3.53589000	2.91723800	-0.58228900
C	-1.80261700	0.73581100	-1.00763400
C	-1.23740500	0.96916300	-2.26372200
C	-1.86316300	0.45514200	-3.40959400

C	-3.10936400	-0.15580600	-3.32500500
C	-3.73827700	-0.23094600	-2.08131900
C	-3.10505600	0.20070500	-0.90563800
H	4.47102300	3.22084900	-0.11933600
H	-4.73424100	-0.65836800	-2.00285200
C	-0.03497500	1.81569500	-2.67925700
C	-0.49040900	3.28488000	-2.98946700
H	-1.11564000	3.63554800	-2.16016100
H	-1.08406200	3.35510700	-3.90691600
H	-1.39208800	1.44533500	-5.28867300
H	-0.90137700	-0.24621600	-5.23677700
C	1.79435800	1.27045700	-0.85293600
H	3.29849300	4.76593900	-1.67067700
H	-3.59611900	-0.55768200	-4.21078900
C	0.81312000	4.10992000	-3.03489700
H	0.66148600	5.15878000	-2.75178700
H	1.24599500	4.11587400	-4.04642500
C	-0.98868900	0.66259900	-4.62928700
C	0.36012900	1.08871100	-4.00548300
H	0.94014500	0.19587900	-3.74790300
H	0.96912500	1.71616100	-4.66591200
C	-3.85836200	0.14965000	0.38824500
C	-4.20023600	-1.09128700	0.97737100
C	-4.32176100	1.35919600	0.96589700
C	-3.72238000	-2.34077300	0.46900800
C	-5.04167300	-1.11909500	2.15390900
C	-5.14442100	1.31741500	2.15398400
C	-4.06711400	-3.52705500	1.06073900
H	-3.03499700	-2.33733200	-0.36563100
C	-5.39384000	-2.38017600	2.72850500
C	-5.48834800	0.08223600	2.70901400
C	-4.92482700	-3.55098900	2.19642300
H	-3.64175700	-4.45105200	0.68277000
H	-6.03331600	-2.38337100	3.60908800
H	-6.11647500	0.05598400	3.59816500
H	-5.18718200	-4.50312100	2.65198200
C	3.78152100	0.76671200	0.67162700
C	3.93450700	1.12520100	2.03201600
C	4.43790200	-0.37982400	0.16152600
C	3.25090000	2.23847900	2.61860900
C	4.79814600	0.34242900	2.88597600
C	5.27869500	-1.16836400	1.03286800
C	3.44362700	2.58174100	3.93064800
H	2.54296700	2.78980300	2.01246800

C	4.97399800	0.73690300	4.24948100
C	5.44490200	-0.78044000	2.36460600
C	4.32553100	1.82938500	4.75801000
H	2.89908200	3.42196800	4.35377700
H	5.63262400	0.13883000	4.87609500
H	6.08994300	-1.37116200	3.01297100
H	4.46405300	2.11527500	5.79815100
C	-4.50106700	3.80004900	0.98623300
H	-4.26074100	4.76228300	0.54065000
C	-4.03551900	2.64733600	0.40904500
H	-3.43511000	2.70260800	-0.49154100
C	-5.29470300	3.75216600	2.16720200
H	-5.65128600	4.67598600	2.61663300
C	-5.60624800	2.54319200	2.72814400
H	-6.21587600	2.48925800	3.62800800
C	4.98536100	-1.90147200	-1.67099800
H	4.87208500	-2.19788400	-2.71063200
C	5.80305000	-2.68079300	-0.80485200
H	6.30773800	-3.56368500	-1.18951300
C	5.94376700	-2.31964900	0.50718800
H	6.56308900	-2.90674300	1.18214800
C	4.33004800	-0.79266900	-1.20488500
H	3.70718900	-0.21504700	-1.87751700
N	-0.58008000	-1.48195500	0.47290100
S	0.12745800	-2.87416700	0.20499000
O	-0.74929400	-3.98008500	0.62017100
O	1.55925700	-2.95191600	0.53146100
C	0.08125800	-3.03237700	-1.66674800
F	-1.16300600	-2.82560900	-2.14255000
F	0.45647700	-4.27266200	-2.02955900
F	0.90333600	-2.16253900	-2.27853400

NTPA-2R-anion-2

0 imaginary frequency

H = -3240.321172

G = -3240.445393

E(M06-2X-DCM) = -3240.859810

O	1.09463000	0.53187300	-0.60821800
O	-1.26343100	0.84898200	0.42193000
P	-0.01648000	-0.26152700	0.37135300
O	0.47975600	-0.43045700	1.75575800
C	2.49256300	4.25598600	0.68852100
C	1.33647300	4.15143700	-0.07838800
C	0.90516500	2.90662200	-0.55595400

C	2. 79309400	1. 83019600	0. 54081300
C	3. 21994800	3. 09917200	0. 96747700
C	-1. 95544000	1. 16031000	-0. 72837500
C	-1. 41256600	2. 06223800	-1. 64654700
C	-2. 00573400	2. 20828600	-2. 90857000
C	-3. 20442500	1. 56856800	-3. 20700200
C	-3. 82497700	0. 80822500	-2. 21447600
C	-3. 22427200	0. 58964000	-0. 96447600
H	4. 13920700	3. 16427200	1. 54344700
H	-4. 79249700	0. 35256400	-2. 40694400
C	-0. 28585900	3. 07968900	-1. 49036200
C	-0. 85655900	4. 44013700	-0. 95690800
H	-1. 49320800	4. 23210600	-0. 08919000
H	-1. 46787700	4. 95925100	-1. 70266200
H	-1. 64170300	4. 08870600	-3. 93730500
H	-1. 00301800	2. 68499400	-4. 78779700
C	1. 59417400	1. 74515900	-0. 19837400
H	2. 83007600	5. 22008600	1. 06262200
H	-3. 66640800	1. 67412700	-4. 18606300
C	0. 38097700	5. 24414300	-0. 50581200
H	0. 15637900	5. 95122600	0. 30213700
H	0. 79682500	5. 83536200	-1. 33531700
C	-1. 16362800	3. 10907100	-3. 78913600
C	0. 14972500	3. 24007600	-2. 98333200
H	0. 82462200	2. 41546400	-3. 23856500
H	0. 68103000	4. 18062200	-3. 16724000
C	-3. 99391600	-0. 14264400	0. 09250100
C	-4. 28180300	-1. 52156000	-0. 04197400
C	-4. 53817600	0. 59134600	1. 17769700
C	-3. 71503500	-2. 32524700	-1. 08140600
C	-5. 15729200	-2. 16878100	0. 91090000
C	-5. 38877300	-0. 07472800	2. 13864300
C	-4. 01374700	-3. 65817500	-1. 19079600
H	-2. 98902800	-1. 88402300	-1. 75173000
C	-5. 46061300	-3. 55624800	0. 74657600
C	-5. 68340200	-1. 43040400	1. 97320300
C	-4. 91124500	-4. 27976800	-0. 27746400
H	-3. 51912600	-4. 24841300	-1. 95507600
H	-6. 12742700	-4. 02561100	1. 46724700
H	-6. 33563800	-1. 92372400	2. 69221700
H	-5. 13678100	-5. 33855000	-0. 38191600
C	3. 65993100	0. 64762900	0. 84446600
C	3. 80829300	0. 19837700	2. 17787600
C	4. 41904700	0. 05337400	-0. 19259700

C	3.03194000	0.72591000	3.25935100
C	4.76565200	-0.84074000	2.48128700
C	5.35071100	-1.00623000	0.11976900
C	3.22144100	0.29605600	4.54592600
H	2.25707000	1.44832000	3.03656100
C	4.93348200	-1.25909600	3.83860400
C	5.50822200	-1.41443900	1.44650200
C	4.19216400	-0.70225800	4.84495700
H	2.60645100	0.70076600	5.34546500
H	5.66168300	-2.03958900	4.04947900
H	6.22178100	-2.20336600	1.67831700
H	4.32522700	-1.03346500	5.87221900
C	-4.85150200	2.67697600	2.42032700
H	-4.65308100	3.73991900	2.53438500
C	-4.30967700	1.99314700	1.36317700
H	-3.69197800	2.51899300	0.64453900
C	-5.67047900	2.00962700	3.37455500
H	-6.08765900	2.56478100	4.21141100
C	-5.93046200	0.67361300	3.23042600
H	-6.55922900	0.14980700	3.94775400
C	5.05980800	-0.13513300	-2.54432900
H	4.95151600	0.18996600	-3.57597200
C	5.96656100	-1.18757300	-2.23223900
H	6.54190100	-1.65719100	-3.02637400
C	6.10662300	-1.60445500	-0.93624700
H	6.79525600	-2.40773300	-0.68248700
C	4.31813600	0.46401000	-1.56026100
H	3.63058600	1.26200000	-1.81538800
N	-0.53752300	-1.40497800	-0.62916700
S	-0.07966100	-2.90732300	-0.84298000
O	-0.81445500	-3.47412000	-1.98677400
O	0.04816000	-3.72312700	0.37290300
C	1.67758400	-2.78833400	-1.47842200
F	1.76438600	-1.96626200	-2.53450300
F	2.11281300	-4.00331300	-1.85820500
F	2.49606500	-2.33278300	-0.51747600

NTPA-2R-anion-3

0 imaginary frequency

H = -3240.320042

G = -3240.442978

E(M06-2X-DCM) = -3240.859289

O	-1.21232700	0.94445900	0.19761000
O	1.14027300	0.13417300	-0.54768500

P	-0.00034200	-0.11895000	0.64779600
O	0.44588100	0.33149700	1.98468800
C	-3.18715400	0.24906900	-3.41825000
C	-1.93665800	0.85612000	-3.40238600
C	-1.32581700	1.20655600	-2.19044100
C	-3.20512600	0.25438800	-0.97403600
C	-3.82977500	0.00221800	-2.20552600
C	1.69397900	1.38394000	-0.69895500
C	1.06180300	2.30126900	-1.54076600
C	1.56622400	3.60517800	-1.64881900
C	2.72776200	3.97815400	-0.98037700
C	3.38821100	3.03056200	-0.19877900
C	2.89103000	1.72722300	-0.03534300
H	-4.82813800	-0.42679600	-2.19894800
H	4.30683300	3.29861800	0.31633900
C	-0.12910400	2.11236700	-2.47421700
C	0.29395400	1.56712900	-3.87621700
H	0.90475900	2.28147200	-4.44005700
H	0.88163100	0.65463200	-3.72707800
H	0.50206000	5.45256300	-2.12830600
H	1.11953600	4.58311400	-3.53152400
C	-1.90160500	0.79603400	-0.98652700
H	-3.66455000	-0.02278700	-4.35691700
H	3.11860800	4.98999600	-1.06294000
C	-1.04203000	1.21511500	-4.57094100
H	-1.43668700	2.06963300	-5.14067300
H	-0.93825200	0.38430000	-5.27873400
C	0.67538900	4.44825600	-2.53402400
C	-0.61076800	3.60048300	-2.60465900
H	-1.19859300	3.77170500	-3.51225800
H	-1.24966000	3.83376900	-1.74492500
C	3.67843400	0.76223700	0.79802800
C	4.44539600	-0.24566800	0.16450200
C	3.74689200	0.92741500	2.20163000
C	4.44177100	-0.44469600	-1.25284600
C	5.29504600	-1.10424400	0.95822900
C	4.62173700	0.08078000	2.98061800
C	5.19866300	-1.42427700	-1.83998000
H	3.81311600	0.18999500	-1.86619200
C	6.06579700	-2.11740900	0.30710100
C	5.36603100	-0.91293200	2.34043800
C	6.02137800	-2.27743300	-1.05147400
H	5.16323000	-1.56032700	-2.91771400
H	6.69081800	-2.76136900	0.92243600

H	6.01827900	-1.55304000	2.93234100
H	6.60918100	-3.05522100	-1.53293400
C	-3.95984400	0.00163700	0.29447700
C	-4.39640800	1.09951200	1.07867600
C	-4.31831400	-1.31704500	0.66577700
C	-4.10043100	2.45987600	0.74324400
C	-5.20064100	0.86524900	2.25690500
C	-5.13585700	-1.53626500	1.83877700
C	-4.54090600	3.50289100	1.51552600
H	-3.51420200	2.65940400	-0.14615200
C	-5.63536300	1.98075700	3.03938700
C	-5.55218400	-0.44246700	2.60120500
C	-5.31580100	3.26374700	2.68572400
H	-4.29475700	4.52416400	1.23520700
H	-6.23102200	1.78173800	3.92815300
H	-6.16246400	-0.61282400	3.48683800
H	-5.65190200	4.10177600	3.29185300
C	3.08673300	2.06988500	4.25615600
H	2.47481200	2.81081300	4.76389300
C	2.97183100	1.90758100	2.90114500
H	2.25818700	2.49897000	2.34209700
C	3.97421400	1.25437300	5.01496400
H	4.04833800	1.39548300	6.09078200
C	4.71087100	0.28288200	4.39381700
H	5.37747200	-0.36104200	4.96396700
C	-4.23041600	-3.73255000	0.32104900
H	-3.83718700	-4.58241600	-0.22778300
C	-5.05910900	-3.94114100	1.45923600
H	-5.32779900	-4.95390800	1.75083000
C	-5.49575300	-2.87313000	2.19612400
H	-6.11576500	-3.02001300	3.07841300
C	-3.87907800	-2.46615200	-0.06577500
H	-3.22755700	-2.32805000	-0.91974300
N	-0.43636900	-1.64825800	0.44411500
S	-0.37135300	-2.66489000	-0.76564900
C	1.46265700	-2.95614200	-1.12265700
O	-0.88360700	-2.15982400	-2.05656500
O	-0.84064600	-3.98643900	-0.32412300
F	1.91161700	-2.12313500	-2.07417500
F	2.21183300	-2.79735800	-0.02391000
F	1.63326900	-4.21316900	-1.57030000

NTPA-2R-anion-4

0 imaginary frequency

H = -3240.317923

G = -3240.442752

E(M06-2X-DCM) = -3240.853867

O	1.36590500	-0.09359400	-0.64910600
O	-0.92807100	0.96914400	-0.02939400
P	0.17893000	-0.16506500	0.51858900
O	0.62393300	0.30847600	1.84806600
C	3.02868900	3.48445600	-2.01032000
C	1.85805100	2.98185700	-2.57039600
C	1.30869200	1.77136900	-2.12536800
C	3.11478000	1.56402900	-0.49804900
C	3.65061100	2.76568300	-0.98990800
C	-1.70158800	0.66466200	-1.12867700
C	-1.15380200	0.69472000	-2.41115600
C	-1.84823900	0.09184700	-3.47008500
C	-3.15047300	-0.36347600	-3.29454300
C	-3.76121900	-0.19586900	-2.04925300
C	-3.05451200	0.30554300	-0.94577500
H	4.57024200	3.13859700	-0.54685400
H	-4.79839000	-0.48947200	-1.90976500
C	0.09049100	1.39063600	-2.96134700
C	-0.31919300	2.80910000	-3.50162700
H	-0.93705300	3.30330600	-2.74261100
H	-0.90813000	2.75103300	-4.42247300
H	-1.31471200	0.69957100	-5.49366200
H	-0.95322900	-0.98871500	-5.13081600
C	1.91944300	1.08580700	-1.07280300
H	3.45375000	4.42369700	-2.35756200
H	-3.69359700	-0.83223200	-4.11195800
C	1.00389000	3.58202300	-3.66392100
H	0.87941500	4.66712100	-3.56175200
H	1.44902400	3.40636000	-4.65468700
C	-0.96742300	0.01966400	-4.70160600
C	0.41967400	0.43955400	-4.15471700
H	0.93544300	-0.44232700	-3.76110800
H	1.05877400	0.91361600	-4.90867700
C	-3.76063800	0.51728400	0.35941900
C	-4.18424600	-0.58073100	1.14431300
C	-4.07968300	1.83772900	0.76698700
C	-3.85945600	-1.93027600	0.80119500
C	-4.95434500	-0.35516500	2.34729600
C	-4.83481200	2.05201400	1.98120700
C	-4.28177600	-2.98172100	1.57116600
H	-3.23721200	-2.10840700	-0.06395600

C	-5.38579800	-1.48107800	3.11643300
C	-5.25655700	0.95243300	2.73369400
C	-5.06421800	-2.75737000	2.73939300
H	-3.98901800	-3.99090000	1.29893300
H	-5.96924900	-1.29602900	4.01620000
H	-5.83136700	1.11987800	3.64320900
H	-5.39104100	-3.60384300	3.33902100
C	3.84602600	0.83720600	0.58798500
C	3.90096400	1.38969400	1.88953500
C	4.55724100	-0.34982200	0.29001700
C	3.15943300	2.55565900	2.26534700
C	4.72034100	0.76132000	2.90031300
C	5.35801100	-0.97935700	1.31529000
C	3.25187700	3.08428300	3.52572600
H	2.49384500	3.00416100	1.53776500
C	4.79211700	1.34759600	4.20283500
C	5.42655800	-0.40212700	2.58585000
C	4.08683700	2.47986500	4.50839200
H	2.66542700	3.96129600	3.78740000
H	5.41806500	0.86351600	4.94986600
H	6.04049300	-0.87442300	3.35109300
H	4.14619400	2.91177600	5.50472500
C	-4.03052900	4.26014300	0.42479900
H	-3.72768100	5.11799900	-0.17055500
C	-3.70588800	2.99466100	0.01028900
H	-3.15287800	2.85486300	-0.91134200
C	-4.75919900	4.46479900	1.63058200
H	-5.00411700	5.47536600	1.94887500
C	-5.14943700	3.38866200	2.38102700
H	-5.71047600	3.52893100	3.30285700
C	5.24039000	-2.10610600	-1.26469100
H	5.18874400	-2.55805500	-2.25150100
C	6.02356400	-2.72459100	-0.24967600
H	6.56840300	-3.63885200	-0.47209200
C	6.07942100	-2.17319800	1.00133400
H	6.67058000	-2.63745100	1.78811400
C	4.53729100	-0.95994100	-1.00455600
H	3.93815600	-0.50799400	-1.78611600
N	-0.45779300	-1.62704900	0.26902400
S	0.24521300	-2.80617500	-0.53996100
O	1.53138600	-3.26814900	0.00817800
O	0.13627700	-2.70415600	-2.00998200
C	-0.93357300	-4.19476300	-0.12266300
F	-1.15721300	-4.30478500	1.19253400

F	-0.40171800	-5.35150800	-0.55513200
F	-2.12588900	-4.04751500	-0.73862600

INT-1

0 imaginary frequencies

H = -3546.208826

G = -3546.348273

E(M06-2X-DCM) = -3546.693470

O	-2.27307500	3.68711400	-1.27637400
O	-3.81353300	2.11985200	0.06436700
P	-2.29564100	2.28074900	-0.47464800
O	-2.02420400	1.12003700	-1.40309900
C	-4.04605000	-2.12619100	-1.72050600
C	-4.50557400	-1.47309300	-0.37490100
H	-5.56749400	-1.22990100	-0.49868900
H	-3.99415900	-0.51273800	-0.25909900
C	-3.03807700	-2.27642300	1.61546400
C	-2.37733900	-1.06196600	1.87113000
C	-2.45277300	-3.46245600	2.09638800
C	-1.17958000	-1.03057100	2.58835200
H	-2.80943500	-0.12361700	1.53764700
C	-1.25150300	-3.43540700	2.80520300
H	-2.94318600	-4.41232500	1.89835200
C	-0.60980700	-2.21946200	3.05342500
H	-0.69367400	-0.07628000	2.77308300
H	-0.81561500	-4.36555000	3.16125500
H	0.32972600	-2.19511800	3.59965100
C	-4.34000800	-2.31271900	0.88394800
C	-2.57932900	-2.61260800	-1.67600500
H	-2.48125800	-3.34892100	-0.86972600
H	-2.35453100	-3.11065300	-2.62919000
N	-1.59857000	-1.54192800	-1.46003400
C	-0.29677800	-1.69812300	-1.30265800
N	0.50697900	-0.64510200	-1.12130600
C	1.89569700	-0.75608100	-0.77098200
C	2.24963100	-1.03501900	0.55078300
C	2.87140700	-0.54297300	-1.74202300
C	3.59727200	-1.12306800	0.89121900
C	4.21941400	-0.62179000	-1.38522600
H	2.58064400	-0.31569600	-2.76137600
C	4.58591500	-0.91485000	-0.07250100
H	5.63358400	-0.97830000	0.19881100
C	5.28126500	-0.33584800	-2.41705700
C	3.99983100	-1.50359500	2.29413200

F	6.42698700	-0.99726100	-2.14704800
F	4.87875200	-0.70129500	-3.65428200
F	5.58198500	0.97833600	-2.46919400
F	5.10024200	-0.83360700	2.69258900
F	3.01922100	-1.26077500	3.18631400
F	4.29263300	-2.82368600	2.37164900
S	0.51785600	-3.27538100	-1.35208500
H	1.47674100	-1.16575100	1.29874100
H	0.10577200	0.30442700	-1.06339200
H	-1.92546900	-0.55174100	-1.39539400
C	-5.35306900	-3.06216200	1.34759900
H	-6.31278300	-3.09941800	0.83846700
H	-0.60120800	-4.00172800	-1.51842100
H	-5.26656200	-3.63831700	2.26453300
N	-1.41724800	2.48474900	0.86800900
S	0.16864600	2.48210000	0.90514700
O	0.66755500	1.88758400	2.15258000
O	0.80055400	2.03536500	-0.36528600
C	0.63762600	4.28658000	1.02687000
F	0.08845000	4.83343600	2.11606700
F	1.96852100	4.39525800	1.11088800
F	0.21534700	4.95265500	-0.05289300
C	-4.24279700	-1.10329100	-2.85809300
H	-3.93353400	-1.52680300	-3.82203000
H	-3.68071700	-0.18018300	-2.68817700
H	-5.30239200	-0.83525900	-2.93929100
C	-4.89647300	-3.37613800	-2.02369500
H	-4.61023900	-3.82508700	-2.98269300
H	-5.95548900	-3.10376700	-2.09054100
H	-4.79793300	-4.13683300	-1.24261300
C	-4.33200600	3.04355700	1.03897400
H	-3.73010900	3.00901300	1.95026700
H	-5.35574200	2.72609500	1.24641000
H	-4.33483300	4.06245000	0.63828700
C	-2.80932400	3.75188400	-2.60705600
H	-2.62177200	4.76650000	-2.96325700
H	-3.88799200	3.55847600	-2.60137500
H	-2.31094300	3.02795900	-3.25722100

INT-1'

0 imaginary frequencies

H = -3546.212781

G = -3546.353592

E(M06-2X-DCM) = -3546.692934

O	0.90783500	-2.24937800	-0.00524300
O	2.66703700	-2.20868400	-1.88065800
P	1.88856000	-1.29971100	-0.82878700
O	1.13186300	-0.12685400	-1.33712400
N	3.16469200	-0.76195900	0.15724200
S	4.53446500	-1.54117900	0.72985000
C	5.82935300	-1.05762600	-0.53956100
F	7.00604300	-1.52065500	-0.12703500
F	5.53059000	-1.57447800	-1.72699000
F	5.87174000	0.27274800	-0.62643400
C	1.70517500	4.17266500	-0.71808100
C	1.88336400	4.08236400	0.83626900
H	2.88477900	4.47539400	1.04635500
H	1.18600200	4.80084400	1.28124500
C	0.45295800	2.26522700	2.07308700
C	-0.56940100	3.15394300	2.44659200
C	0.20699800	0.88766700	2.23624200
C	-1.77457400	2.68878300	2.97267700
H	-0.42902400	4.22453700	2.34421500
C	-0.99716600	0.41977300	2.75597000
H	0.96282000	0.16800700	1.93795300
C	-1.99575400	1.32171200	3.13012700
H	-2.54574500	3.40168400	3.24952300
H	-1.16727000	-0.64996000	2.84538300
H	-2.94053200	0.96083500	3.52626700
C	1.77246500	2.75135400	1.57326900
C	0.24844200	3.96087300	-1.19641200
H	0.17282400	4.29651900	-2.24228100
H	-0.43280500	4.59348800	-0.62145700
N	-0.22469200	2.59159200	-1.09095800
C	-1.53487100	2.23129300	-1.05464300
N	-1.67254500	0.85511000	-1.04364600
C	-2.75896200	0.03321000	-0.71837800
C	-4.11226100	0.35377300	-0.91515000
C	-2.43448100	-1.22594900	-0.19092500
C	-5.09559900	-0.57124800	-0.56209600
C	-3.43079000	-2.13478300	0.15417200
H	-1.39330500	-1.48585400	-0.02977100
C	-4.77615100	-1.81961600	-0.02351300
H	-5.55323200	-2.52472200	0.24301100
C	-3.00179200	-3.44649400	0.74695300
C	-6.54597000	-0.19059800	-0.71860500
F	-2.20504800	-4.14882900	-0.10405800
F	-4.03754700	-4.24091000	1.07124100

F	-2.26054200	-3.26626300	1.87384700
F	-7.32523300	-1.27492400	-0.94071600
F	-6.73873400	0.66356500	-1.74444400
F	-7.02404800	0.41173600	0.39468300
S	-2.79638900	3.34530700	-1.02816000
C	2.05844800	5.62843000	-1.10174700
H	3.08162200	5.87560400	-0.79710800
H	1.98650800	5.77727400	-2.18507000
H	1.38161000	6.34414700	-0.61984400
C	2.68450800	3.23364500	-1.44674700
H	2.58524200	3.34095000	-2.53366700
H	3.72015100	3.48020800	-1.18278600
H	2.53032000	2.17877700	-1.20072500
H	-4.38164400	1.31320800	-1.33274900
C	2.90261300	2.07515900	1.87171500
H	-0.78691500	0.35199700	-1.03945100
H	3.87784800	2.44160800	1.56102500
H	2.90453500	1.20434700	2.52152800
O	4.34101600	-2.98013100	0.62240900
H	0.46067600	1.85139900	-1.19951500
O	4.91868500	-0.87409100	1.96555000
H	3.04779500	0.18902000	0.53019600
C	1.23547400	-3.53340600	0.58497100
H	1.79634500	-3.38095000	1.50848400
H	0.27475300	-4.00436700	0.78835000
H	1.82690000	-4.13640200	-0.10655000
C	1.95680200	-2.76593700	-3.01486700
H	1.52700800	-1.96181900	-3.61662000
H	2.70320400	-3.31263100	-3.59020200
H	1.17028300	-3.44681000	-2.67768300

INT-1''

0 imaginary frequencies

H = -3546.197632

G = -3546.336646

E(M06-2X-DCM) = -3546.68586

O	-4.93135700	2.24783900	-0.37640400
O	-5.07343300	1.29263700	2.02579800
P	-4.21823300	1.30143900	0.68167300
O	-4.43251400	-0.15210300	0.08589000
N	-2.76257700	1.80178400	1.03151500
S	-1.40915700	1.76760400	0.17158400
C	-1.45145900	3.36126700	-0.81020200
F	-0.30447500	3.47840900	-1.48440300

F	-2.47052500	3.33919300	-1.67366400
F	-1.59140600	4.40045000	0.01105200
C	-2.36858100	-3.77164000	-1.58365900
C	-2.58181700	-4.13716200	-0.07273000
H	-3.61648000	-4.48928900	0.01072700
H	-1.95327300	-5.01077000	0.13711300
C	-1.00169100	-2.81174600	1.53259100
C	-0.00148100	-3.79912400	1.56821900
C	-0.67945600	-1.53293700	2.02346900
C	1.26690500	-3.51700400	2.07377200
H	-0.20783700	-4.80243400	1.21051800
C	0.59150100	-1.24566000	2.51382900
H	-1.41972600	-0.74010900	1.99045600
C	1.57383900	-2.23847700	2.54182600
H	2.02200800	-4.29767000	2.08469900
H	0.81692300	-0.23607100	2.84330900
H	2.57592500	-2.00956200	2.89354900
C	-2.37221100	-3.11070900	1.03201600
C	-0.89086200	-3.54126200	-1.98061500
H	-0.81363200	-3.59528400	-3.07631500
H	-0.26766500	-4.35327200	-1.59380000
N	-0.32119100	-2.28355600	-1.52439100
C	1.01056300	-2.01346900	-1.54104700
N	1.27950600	-0.71187000	-1.17640900
C	2.48700800	-0.11150700	-0.78741400
C	3.53648600	-0.80560600	-0.17410100
C	2.58955900	1.27896200	-0.94483300
C	4.65360200	-0.10547500	0.28291400
C	3.71359200	1.96059800	-0.48803900
H	1.77901500	1.82844900	-1.40997700
C	4.75975300	1.27600800	0.13305400
H	5.62911200	1.80775600	0.49924100
C	3.82768300	3.44384000	-0.71658000
C	5.70449100	-0.87305700	1.03894100
F	2.61727600	4.03644500	-0.82211900
F	4.50168100	3.72372200	-1.85741800
F	4.49372600	4.05591200	0.28823600
F	6.83798000	-0.16045900	1.21225700
F	6.03647400	-2.02395000	0.41862100
F	5.26239800	-1.21712100	2.27906600
S	2.16517200	-3.14686800	-2.01112300
H	3.47070200	-1.87672300	-0.04523200
C	-3.45413400	-2.55193400	1.62512500
H	0.47095900	-0.09775600	-1.10405700

H	-4.46271900	-2.83657600	1.33220600
H	-3.36266200	-1.93236500	2.51383000
O	-1.40438200	0.69972400	-0.85872300
H	-0.95116400	-1.53547500	-1.26040700
O	-0.25732700	1.88207300	1.05999100
H	-3.93906900	-0.88825000	0.53395200
C	-2.81828600	-5.02090400	-2.37760600
H	-3.86168300	-5.27159900	-2.15511800
H	-2.20218600	-5.89399600	-2.13153400
H	-2.73786100	-4.84806900	-3.45639000
C	-3.25735300	-2.58939700	-2.00955200
H	-4.31213800	-2.80132400	-1.79557500
H	-3.16678600	-2.41395500	-3.08802300
H	-3.00845100	-1.65105900	-1.50585800
C	-6.24546300	1.95281600	-0.91102200
H	-6.20800800	1.03419700	-1.49977800
H	-6.50162600	2.80088100	-1.54556600
H	-6.97229200	1.85586200	-0.09997600
C	-4.91952200	2.33310700	3.02454100
H	-3.87297200	2.40770100	3.32434600
H	-5.54290800	2.02674500	3.86438500
H	-5.26845800	3.29023900	2.62734400

TS-E-1

1 imaginary frequencies

H = -3546.193030

G = -3546.327946

E(M06-2X-DCM) = -3546.664627

O	-3.73926100	2.77126700	-0.72825000
O	-4.52349800	1.39153900	1.29520800
P	-3.28388200	1.58500800	0.27957300
O	-3.08694000	0.27716500	-0.44329900
C	-3.43103100	-3.22227800	-1.46941900
C	-3.00446000	-3.34064500	0.03196900
H	-3.66057200	-4.09560400	0.49501900
H	-3.26144600	-2.40249700	0.52615500
C	-0.96735200	-3.03281300	1.56273700
C	-1.20633600	-1.66206600	1.81339900
C	-0.04804300	-3.71203000	2.39646700
C	-0.51631600	-0.98974100	2.81880300
H	-1.88061900	-1.09395600	1.18142200
C	0.61339800	-3.04489100	3.42097500
H	0.11609300	-4.77682400	2.26461600
C	0.39245400	-1.67930700	3.62504000

H	-0.66853400	0.07740700	2.94436200
H	1.30752100	-3.58709300	4.05621200
H	0.93001600	-1.15302800	4.40850400
C	-1.59838400	-3.72597500	0.43103100
C	-2.33073300	-2.56249800	-2.36073800
H	-1.68084200	-3.32128300	-2.79539100
H	-2.83002500	-2.05271200	-3.19490600
N	-1.47237200	-1.58860600	-1.68628600
C	-0.13115600	-1.58656300	-1.68835000
N	0.48354300	-0.46013300	-1.28309200
C	1.85969500	-0.30520300	-0.94276200
C	2.47902900	-1.13668000	-0.00825900
C	2.55856400	0.76832100	-1.49844500
C	3.81185400	-0.91385900	0.33480900
C	3.88792500	0.98727700	-1.13761500
H	2.06165600	1.42940300	-2.19857500
C	4.52527200	0.14405000	-0.22803500
H	5.55955400	0.31469400	0.04520500
C	4.62842900	2.17552900	-1.69628500
C	4.48683500	-1.85514400	1.29732600
F	4.50330800	3.25949600	-0.90236300
F	5.95153100	1.92268800	-1.81490500
F	4.16849500	2.52089700	-2.91828500
F	4.93087800	-2.97119600	0.67388000
F	5.55260000	-1.28654500	1.89813600
F	3.64041500	-2.26539400	2.27089900
S	0.79017500	-2.98583700	-2.18146900
H	1.92336900	-1.93994100	0.45837900
H	-0.06915900	0.40500300	-1.15103700
H	-1.96091300	-0.77076400	-1.27470300
C	-0.87003100	-4.69073000	-0.26875200
H	-1.39961900	-5.38129800	-0.91915400
H	-0.17853900	-3.94328900	-1.17632300
H	0.01649900	-5.11035000	0.20529900
N	-2.09142500	2.18562800	1.19897900
S	-0.64463300	2.53415500	0.66499000
O	0.38945600	2.18994800	1.64783800
O	-0.39713200	2.12675100	-0.75206900
C	-0.61837000	4.39989200	0.57663800
F	-0.84568500	4.91725900	1.78868800
F	0.58091600	4.80891700	0.14844400
F	-1.55578400	4.84329300	-0.26656000
C	-4.71290900	-2.35734000	-1.48569200
H	-5.48442700	-2.80184300	-0.84530500

H	-5.12093000	-2.30214900	-2.50232900
H	-4.51452700	-1.34229800	-1.13084700
C	-3.78856000	-4.58320600	-2.10571600
H	-4.13568000	-4.43785000	-3.13581100
H	-4.60209000	-5.06588500	-1.55236800
H	-2.94675200	-5.28057000	-2.14674500
C	-4.63060900	2.47157500	-1.81099300
H	-4.21341200	1.68643400	-2.44794900
H	-4.74158500	3.39479600	-2.38293000
H	-5.60976300	2.15404700	-1.43449700
C	-4.88593000	2.45044400	2.19718300
H	-4.05090900	2.68389900	2.86268400
H	-5.73802300	2.08309800	2.77265400
H	-5.17547300	3.34922400	1.64249600

INT-2

0 imaginary frequencies

H = -3546.193130

G = -3546.330877

E(M06-2X-DCM) = -3546.673294

O	-3.88435500	2.28346700	-1.11042600
O	-4.72330200	0.98356400	0.94784400
P	-3.40465700	1.25137000	0.04490700
O	-2.98334800	-0.07840400	-0.51934100
C	-3.21646200	-3.55123800	-1.20508900
C	-2.99241500	-3.33050900	0.34353100
H	-3.58087500	-4.09924400	0.86953300
H	-3.42166900	-2.36245300	0.59239100
C	-1.03841900	-2.46867200	1.79080300
C	-1.77886100	-1.35250500	2.27056400
C	0.32520100	-2.57587800	2.18922900
C	-1.18058300	-0.39590900	3.07508500
H	-2.81580300	-1.21663300	1.99503200
C	0.92273600	-1.60390800	2.97438100
H	0.92991700	-3.40397700	1.84047400
C	0.17295800	-0.50536500	3.41230700
H	-1.74879900	0.47073700	3.39087600
H	1.97797100	-1.68400500	3.21675100
H	0.64342900	0.27853500	3.99694400
C	-1.59416900	-3.42834000	0.87418700
C	-1.98944000	-3.02850900	-2.01783500
H	-1.33317600	-3.84918000	-2.30946600
H	-2.35122200	-2.55586500	-2.94080300
N	-1.17111700	-2.07348700	-1.27719400

C	0.19481500	-1.97555900	-1.40204900
N	0.69434900	-0.78211200	-0.98515800
C	2.05724100	-0.43660000	-0.79056900
C	2.94225100	-1.27201900	-0.10655600
C	2.48959200	0.82473600	-1.21801800
C	4.24673600	-0.84851500	0.14534100
C	3.79978200	1.23035600	-0.96886900
H	1.79705500	1.48788400	-1.72123500
C	4.69023400	0.39903900	-0.28781600
H	5.70571400	0.72151800	-0.09340400
C	4.24685700	2.60837400	-1.38515600
C	5.15620900	-1.77400800	0.90652000
F	4.07614900	3.50845600	-0.39282900
F	5.56067700	2.62463700	-1.70838800
F	3.55887200	3.05849200	-2.45517900
F	5.51925400	-2.84762700	0.17247900
F	6.28611900	-1.16347800	1.31514800
F	4.53694500	-2.26146900	2.01664000
S	1.14577100	-3.26601900	-1.96605000
H	2.61292500	-2.24115900	0.23977300
H	0.05248900	0.00882900	-0.83768200
H	-1.68273500	-1.22387800	-0.98310700
C	-0.83797500	-4.66902700	0.56411600
H	-1.50000000	-5.47582400	0.25293400
H	-0.13417300	-4.47320500	-0.27827300
H	-0.23133000	-5.01483100	1.40276600
N	-2.42109600	2.08453300	1.02803700
S	-0.92333300	2.46137100	0.68114700
O	-0.07254800	2.42111700	1.87679200
O	-0.40197100	1.81307000	-0.55677900
C	-0.98935700	4.26948600	0.21443600
F	-1.47464500	4.98872100	1.23225800
F	0.24402200	4.70051700	-0.07201200
F	-1.77146100	4.44931500	-0.85479100
C	-4.49180900	-2.75973200	-1.57248000
H	-5.34542600	-3.10439400	-0.97599900
H	-4.74258800	-2.91785100	-2.62814300
H	-4.35514400	-1.69001300	-1.39534200
C	-3.46434300	-5.02572400	-1.58908600
H	-3.68132100	-5.09478800	-2.66155500
H	-4.33224700	-5.42956200	-1.05503200
H	-2.60728100	-5.67671600	-1.39627600
C	-4.59249100	1.78501900	-2.25378600
H	-4.00143700	1.02457500	-2.77182400

H	-4.75538800	2.64095500	-2.91152000
H	-5.55941600	1.35996000	-1.96068600
C	-5.33570800	2.07157100	1.66001300
H	-4.62814900	2.50751100	2.37035400
H	-6.19261300	1.64921200	2.18916000
H	-5.67749900	2.84518100	0.96452100

INT-3

0 imaginary frequencies

H = -3546.213997

G = -3546.346872

E(M06-2X-DCM) = -3546.706010

O	-1.21403300	2.67541300	-1.92499800
O	-3.68930500	2.82046200	-1.23437700
P	-2.27514400	2.18560600	-0.79513000
O	-2.43554800	0.68466900	-0.82310000
C	-4.29732200	-2.38036900	-1.15689100
C	-4.00311100	-2.53954800	0.36765000
H	-4.56117900	-3.36925200	0.81230200
H	-4.30476700	-1.63407200	0.89871500
C	-1.95503100	-2.23363200	1.89370400
C	-2.22418600	-0.90941200	2.27893300
C	-1.23083200	-3.04574800	2.78032200
C	-1.77949500	-0.41110900	3.50222600
H	-2.75862100	-0.23795200	1.61282700
C	-0.79974700	-2.55290700	4.01264500
H	-1.00200600	-4.07464600	2.52943800
C	-1.07112500	-1.23546000	4.37685500
H	-1.96073900	0.62883000	3.75234000
H	-0.24524300	-3.20416200	4.68271200
H	-0.72468500	-0.84717500	5.33028800
C	-2.48531600	-2.77724200	0.56773100
C	-2.89354400	-2.19443300	-1.79507300
H	-2.53285600	-3.08389900	-2.30919100
H	-2.83321800	-1.34011800	-2.47018700
N	-1.94287300	-1.91428300	-0.65195700
C	-0.48391400	-2.04056500	-0.99138900
N	0.23264400	-1.10500500	-0.35202100
C	1.65074000	-0.94751300	-0.43585100
C	2.51878900	-2.01285300	-0.18757400
C	2.15201400	0.32554800	-0.70925100
C	3.89437300	-1.79605800	-0.22790000
C	3.53264100	0.52868200	-0.73425300
H	1.47342500	1.15158700	-0.87896700

C	4.41014000	-0.52704400	-0.49970300
H	5.48084300	-0.36402700	-0.52041000
C	4.05633000	1.92421900	-0.96682900
C	4.83626300	-2.95420300	-0.02144200
F	3.94377800	2.68475200	0.14178400
F	5.36073400	1.91695100	-1.31913500
F	3.37196200	2.54944300	-1.94871400
F	5.16109300	-3.54416100	-1.19348100
F	5.99152500	-2.55992700	0.55538700
F	4.29104300	-3.90887800	0.76412400
S	0.06013200	-3.19548300	-2.04441200
H	2.12981200	-2.99485800	0.04582000
H	-0.22711600	-0.33912900	0.16373400
H	-2.11190000	-0.89506100	-0.44525600
C	-2.13279200	-4.25013800	0.33635100
H	-2.47653700	-4.60500100	-0.63536400
H	-1.06083100	-4.44228000	0.39481100
H	-2.63440200	-4.84398500	1.10583800
N	-1.86842700	2.94558400	0.56902000
S	-0.64424600	2.56148800	1.49576500
O	-0.93116500	2.83821900	2.90527200
O	-0.01850900	1.24980800	1.16924200
C	0.69786700	3.78247200	1.03909800
F	0.26113700	5.03623900	1.17904400
F	1.75787900	3.59653700	1.83053900
F	1.07648900	3.59794100	-0.23715000
C	-5.18585800	-1.14454300	-1.40145600
H	-6.13579300	-1.24826800	-0.86394500
H	-5.41864500	-1.04087800	-2.46819000
H	-4.69423600	-0.22492100	-1.07212700
C	-4.99209200	-3.61876100	-1.75501700
H	-5.11179200	-3.51050600	-2.83957600
H	-5.99212900	-3.73947400	-1.32366200
H	-4.43433100	-4.54314300	-1.57135500
C	-1.31472300	2.15931800	-3.25993200
H	-1.17409900	1.07373200	-3.26774800
H	-0.52057900	2.63721600	-3.83646000
H	-2.28736900	2.40419000	-3.70052300
C	-3.90956700	4.23947900	-1.13289100
H	-3.79367200	4.56608900	-0.09698700
H	-4.93130500	4.41277500	-1.47586100
H	-3.20776900	4.78641100	-1.77126100

l imaginary frequencies

H = -3546.207282

G = -3546.339078

E(M06-2X-DCM) = -3546.697169

O	-3.03816300	2.48416000	-1.87002500
O	-4.44364900	0.86784700	-0.42848200
P	-2.95917000	1.44224800	-0.65707200
O	-2.13948600	0.23865900	-1.18746600
C	-3.44268400	-3.36573600	-1.05436200
C	-3.11811400	-3.28344300	0.46522500
H	-3.32806300	-4.22395400	0.98493200
H	-3.74423100	-2.52347700	0.93587900
C	-1.36256800	-2.09861400	1.90056000
C	-2.18245300	-1.00291400	2.21890300
C	-0.34165000	-2.42838800	2.80494000
C	-1.99233900	-0.26781500	3.38712300
H	-2.98395400	-0.70459100	1.55031200
C	-0.15111000	-1.69774400	3.97927500
H	0.31797300	-3.26531500	2.60892900
C	-0.97457600	-0.61427400	4.27585600
H	-2.62418000	0.59106800	3.58969100
H	0.64909400	-1.97933600	4.65825600
H	-0.82161400	-0.03732400	5.18307500
C	-1.61837600	-2.92444700	0.63321200
C	-2.17280300	-2.79719700	-1.73626300
H	-1.57022300	-3.58645400	-2.18809600
H	-2.39526200	-2.06813500	-2.51950500
N	-1.36558700	-2.10675400	-0.67605200
C	0.04649100	-1.92004300	-1.03016900
N	0.63908800	-0.99901200	-0.23981100
C	2.01357700	-0.61955200	-0.31268400
C	3.02628900	-1.55220900	-0.07671400
C	2.33280400	0.71452400	-0.56529600
C	4.35776900	-1.14450900	-0.10322200
C	3.67172400	1.11110100	-0.58345400
H	1.54366700	1.43631700	-0.73057400
C	4.68973700	0.18821000	-0.35678400
H	5.72722000	0.50039200	-0.37415400
C	4.01130500	2.54146500	-0.91635100
C	5.44836400	-2.13230500	0.21938100
F	3.07968700	3.39817600	-0.44900600
F	5.20348800	2.90661400	-0.39675200
F	4.08798800	2.73243600	-2.25390100
F	6.58553100	-1.85819200	-0.45532200

F	5.75917500	-2.11410700	1.53690300
F	5.08713800	-3.39790300	-0.08193400
S	0.80420600	-2.72390700	-2.27488400
H	2.77716900	-2.58719300	0.12000200
H	0.06283100	-0.37541200	0.33081200
H	-1.89296700	-0.75471900	-0.75424700
C	-0.77452300	-4.21042400	0.59313100
H	-0.98133800	-4.79176400	-0.30714800
H	0.29898400	-4.00936300	0.60636500
H	-1.01878600	-4.83131200	1.46017400
N	-2.56373300	2.23164300	0.65971300
S	-1.12861300	2.53428700	1.29339400
O	-1.29035900	3.07862700	2.63782400
O	-0.15623800	1.44219800	1.07625500
C	-0.43965000	3.92956200	0.25442800
F	-1.29967200	4.94629200	0.19315700
F	0.71027000	4.35168400	0.77944500
F	-0.20861700	3.48074100	-0.99360500
C	-4.68750100	-2.52206300	-1.38771900
H	-5.56281600	-2.89682000	-0.84299900
H	-4.91742800	-2.57547400	-2.45902900
H	-4.55089600	-1.46962300	-1.12273200
C	-3.69361900	-4.81292500	-1.52012600
H	-3.83909200	-4.85357900	-2.60639100
H	-4.59683500	-5.21852000	-1.04928300
H	-2.85915400	-5.47732400	-1.27179500
C	-3.26998600	2.03630400	-3.22215200
H	-2.44647900	1.40035400	-3.55436800
H	-3.31857600	2.93963800	-3.83096600
H	-4.21639600	1.49078000	-3.29017200
C	-5.45461400	1.68493700	0.20442700
H	-5.11443600	2.00343600	1.19172300
H	-6.34052400	1.05402300	0.28536700
H	-5.67470700	2.56018600	-0.41377100

1

0 imaginary frequencies

H = -1957.923291

G = -1958.016713

E(M06-2X-DCM) = -1958.271552

C	-4.76464200	1.39964300	0.32479000
C	-4.42093900	0.67216600	-0.99292300
H	-4.50598800	1.37977500	-1.82621800
H	-5.09457300	-0.16331300	-1.20534500

C	-2.85342800	-1.30919200	-0.55783600
C	-2.52963400	-1.76631300	0.72894000
C	-3.13549200	-2.27144500	-1.54252600
C	-2.47992400	-3.13292400	1.02009400
H	-2.31634300	-1.04719800	1.51379300
C	-3.09283300	-3.63431100	-1.25242400
H	-3.39910500	-1.95951100	-2.54853300
C	-2.76063000	-4.07327700	0.03086700
H	-2.22357500	-3.45538700	2.02557900
H	-3.31668500	-4.35502200	-2.03427300
H	-2.72208300	-5.13546000	0.25488300
C	-2.93585400	0.19291700	-0.90504900
C	-3.39986700	1.99775000	0.71453100
H	-3.25210000	2.99081400	0.26974400
H	-3.27211700	2.11292200	1.79377000
N	-2.38757200	1.06503100	0.18728300
C	-1.06434400	1.28075900	0.46918800
N	-0.21830900	0.28897500	0.00259200
C	1.18725500	0.21531600	0.03772100
C	2.02522300	1.32156400	-0.16267700
C	1.75764800	-1.05410100	0.19801100
C	3.40698300	1.14273300	-0.18086700
C	3.14223400	-1.21616700	0.16832200
H	1.11829400	-1.91889600	0.34960000
C	3.98078300	-0.11903900	-0.01451000
H	5.05675600	-0.24279300	-0.03044400
C	3.72958200	-2.58132700	0.41079100
C	4.30035900	2.32242000	-0.46962300
F	2.93348700	-3.56140300	-0.07555600
F	4.94189900	-2.71738100	-0.16709200
F	3.89039800	-2.82844800	1.73100800
F	5.49468000	2.20684000	0.15247400
F	4.55862200	2.43057000	-1.79506300
F	3.74605100	3.48718200	-0.07923000
S	-0.53960000	2.61196200	1.35339500
H	1.60143000	2.30665400	-0.29389200
H	-0.66133500	-0.60513000	-0.17560800
C	-2.24252900	0.50046200	-2.25548500
H	-2.20739500	1.58408500	-2.40488600
H	-1.22411700	0.11235600	-2.31513400
H	-2.81791500	0.07058000	-3.08068700
C	-5.28695200	0.43154000	1.40344100
H	-6.22461700	-0.03568600	1.07933300
H	-5.48765300	0.97058700	2.33693400

H	-4.57760600	-0.36968200	1.62481600
C	-5.80585100	2.50787000	0.10115700
H	-5.98966400	3.06630300	1.02679000
H	-6.76335600	2.08419200	-0.22421000
H	-5.47458800	3.22186400	-0.66192900

INT-4

0 imaginary frequencies

H = -5198.743377

G = -5198.936847

E(M06-2X-DCM) = -5199.589909

O	1.73030800	-2.28461700	-0.21529400
O	3.12428800	-0.14038200	0.18923000
P	1.59238200	-0.65568700	-0.05080800
O	0.80199700	-0.28148200	1.16772700
C	3.31988300	-4.43553400	3.01251800
C	4.15502000	-3.82663400	2.08207800
C	3.62107300	-3.17020900	0.96285600
C	1.36648500	-3.66941900	1.75017800
C	1.94037000	-4.37802500	2.82050600
C	4.08348200	-0.33523700	-0.80935800
C	4.70106300	-1.57907300	-0.93356500
C	5.52746400	-1.82472400	-2.04166100
C	5.82941100	-0.80868700	-2.94139300
C	5.30676100	0.46531700	-2.72171100
C	4.41814100	0.73099700	-1.66661800
H	1.27677000	-4.87455800	3.52238400
H	5.56782500	1.28009200	-3.39049600
C	4.74254500	-2.77934400	0.00749200
C	5.93335800	-2.65180700	1.01836300
H	5.89168100	-1.66131800	1.48616300
H	6.90790200	-2.74902400	0.53024700
H	7.03024300	-3.36904000	-1.78190300
H	5.87074000	-3.72398300	-3.05765700
C	2.23848800	-3.03829800	0.84091200
H	3.73061200	-4.95588700	3.87416600
H	6.47363600	-0.99531300	-3.79695700
C	5.66540800	-3.73983500	2.07983400
H	6.07312200	-3.48174000	3.06401200
H	6.11854300	-4.69941300	1.79358300
C	5.97263900	-3.27119100	-2.06474300
C	5.04607100	-3.92407500	-1.01604200
H	4.10632800	-4.22896200	-1.49054200
H	5.48209700	-4.80733900	-0.53862900

C	3. 92314800	2. 12903400	-1. 47086300
C	3. 10853900	2. 73966500	-2. 45561500
C	4. 36698700	2. 87551400	-0. 34981600
C	2. 60674700	2. 03212800	-3. 59527100
C	2. 74110100	4. 13132200	-2. 31559800
C	3. 97310600	4. 25963400	-0. 21323000
C	1. 83218500	2. 65722500	-4. 53594200
H	2. 81318000	0. 97331900	-3. 68679600
C	1. 93514400	4. 74675900	-3. 32426200
C	3. 17620800	4. 84892700	-1. 19852900
C	1. 49868700	4. 03539500	-4. 40842200
H	1. 44416700	2. 08792800	-5. 37548700
H	1. 67290800	5. 79521800	-3. 20369600
H	2. 89018600	5. 89355200	-1. 09441000
H	0. 88265300	4. 51222800	-5. 16611500
C	-0. 12325700	-3. 65597300	1. 61669300
C	-0. 91382800	-3. 06100700	2. 63189900
C	-0. 74504100	-4. 33139600	0. 53718000
C	-0. 34980100	-2. 34063500	3. 73481200
C	-2. 35404200	-3. 17083400	2. 57447600
C	-2. 18763200	-4. 40496100	0. 47534500
C	-1. 13954900	-1. 81288000	4. 72426600
H	0. 72467500	-2. 21013900	3. 77641400
C	-3. 14247400	-2. 60186600	3. 62407700
C	-2. 95134800	-3. 83580000	1. 49947600
C	-2. 55676000	-1. 95003800	4. 67644300
H	-0. 67962400	-1. 28656900	5. 55717900
H	-4. 22345000	-2. 70836500	3. 56973200
H	-4. 03564800	-3. 91048700	1. 45560300
H	-3. 16782300	-1. 53951300	5. 47648400
C	5. 64403400	3. 08445600	1. 72725500
H	6. 30057500	2. 64427900	2. 47341300
C	5. 22753600	2. 33311800	0. 65912100
H	5. 56206900	1. 30644000	0. 56520200
C	5. 23442200	4. 44155300	1. 86676300
H	5. 57726500	5. 02416500	2. 71797200
C	4. 42497700	5. 00829700	0. 91892900
H	4. 11140000	6. 04590300	1. 00447300
C	-0. 63918000	-5. 62718100	-1. 53132600
H	-0. 05147300	-6. 10930600	-2. 30773000
C	-2. 06026000	-5. 66909800	-1. 60183300
H	-2. 54350500	-6. 17412900	-2. 43364500
C	-2. 81076800	-5. 07819300	-0. 62246100
H	-3. 89597300	-5. 09941200	-0. 66360800

C	-0.00614100	-4.98537100	-0.49983800
H	1.07653200	-4.96958900	-0.46279400
C	0.73650900	2.43602000	3.74157900
C	1.27677300	3.18203100	2.47827600
H	2.32991800	3.40924100	2.67623300
H	1.27845700	2.47757300	1.64063700
C	-0.56682800	4.42385100	1.11468100
C	-0.49962200	3.64371900	-0.05414600
C	-1.71493500	5.21071800	1.31907500
C	-1.53125900	3.66368300	-0.99391600
H	0.37899800	3.03982500	-0.25980400
C	-2.75054400	5.22910500	0.38443200
H	-1.79495100	5.80492100	2.22561500
C	-2.66112900	4.45893400	-0.77809300
H	-1.44109500	3.05312200	-1.88762600
H	-3.62888100	5.84354500	0.56638700
H	-3.47148500	4.46712800	-1.50251500
C	0.56729600	4.47003400	2.08438200
C	-0.75813600	2.05566400	3.61616200
H	-1.34852700	2.97559500	3.56268100
H	-1.04602100	1.51225700	4.52799900
N	-1.10331600	1.23676100	2.44311700
C	-2.32560500	1.08085900	1.96317700
N	-2.54205300	0.44922100	0.80448800
C	-3.80323500	0.32047800	0.14728900
C	-4.56800700	1.44801600	-0.15524200
C	-4.22625200	-0.94780100	-0.25617400
C	-5.78834000	1.29556300	-0.81615800
C	-5.44287600	-1.08216300	-0.92394200
H	-3.60145700	-1.81022800	-0.05511800
C	-6.23522800	0.03342800	-1.20028600
H	-7.18008600	-0.07977500	-1.71600600
C	-5.88846400	-2.46230100	-1.33733300
C	-6.58259900	2.53417700	-1.14147100
F	-7.09873700	-2.45117700	-1.93073900
F	-5.97692100	-3.29172700	-0.26385800
F	-5.01696700	-3.03201000	-2.19252000
F	-7.78845300	2.24346300	-1.66774900
F	-5.93071300	3.31918200	-2.03136800
F	-6.78771200	3.28801300	-0.03779200
S	-3.76018100	1.67907700	2.83315500
H	-4.19987000	2.43917200	0.08715600
H	-1.75390400	0.02429200	0.28464900
H	-0.34180000	0.72756700	1.94863200

C	0.97589900	5.65196200	2.57526000
H	1.81205900	5.72125000	3.26566000
H	-3.15487400	1.72196600	4.03403900
H	0.51055600	6.58774700	2.27849600
N	1.17050000	-0.10283300	-1.50496300
S	-0.26516100	-0.28192400	-2.14485000
O	-0.69741800	0.90927600	-2.88332000
O	-1.26065500	-0.90805700	-1.22717800
C	0.00272700	-1.57308600	-3.46799100
F	0.89511200	-1.12562400	-4.36212900
F	-1.15178400	-1.81699000	-4.09723000
F	0.45791700	-2.71011800	-2.93555600
C	1.60942400	1.18815200	3.98499300
H	1.26917400	0.64617900	4.87671100
H	1.60169000	0.50108100	3.13546400
H	2.64827600	1.49181300	4.15732300
C	0.82746800	3.33952200	4.98887300
H	0.47618600	2.80933200	5.88291700
H	1.86886200	3.62912700	5.16695300
H	0.24051700	4.25653700	4.87802400

INT-4'

0 imaginary frequencies

H = -5198.748664

G = -5198.944452

E(M06-2X-DCM) = -5199.586957

C	0.10562400	-2.25127100	4.51449800
C	0.23377400	-0.89102700	5.27818100
H	-0.72748300	-0.72281900	5.77867300
H	0.96871900	-1.03889500	6.07760300
C	2.02594300	0.69388300	4.26800000
C	2.99986900	0.45791700	5.25381000
C	2.44202900	1.28897000	3.06412900
C	4.33377700	0.80869700	5.04691600
H	2.71682700	0.02071100	6.20643200
C	3.77571700	1.63001400	2.85149900
H	1.71541500	1.45741800	2.27496300
C	4.72887000	1.39206500	3.84376100
H	5.06498500	0.61911100	5.82817900
H	4.06969500	2.07115400	1.90359000
H	5.77123700	1.64856700	3.67550100
C	0.58931400	0.36706200	4.50258300
C	1.39558600	-2.67241500	3.76521000
H	1.34893000	-3.75245500	3.56723800

H	2. 27049300	-2. 51262400	4. 40305100
N	1. 61528900	-1. 97402800	2. 50611900
C	2. 73856100	-2. 11361900	1. 75494800
N	2. 63761200	-1. 41928000	0. 56452200
C	3. 48442200	-1. 26413300	-0. 53587400
C	4. 78859900	-1. 76857700	-0. 65631100
C	2. 95063700	-0. 51272900	-1. 60356400
C	5. 51736000	-1. 52472400	-1. 82349700
C	3. 69631100	-0. 27955600	-2. 75170900
H	1. 95288900	-0. 09609800	-1. 51786500
C	4. 99274700	-0. 78490000	-2. 88009700
H	5. 58080400	-0. 59217500	-3. 76921900
C	3. 09610100	0. 50026700	-3. 88792900
C	6. 89315100	-2. 12794000	-1. 95393900
F	2. 66582700	-0. 30160300	-4. 89320500
F	3. 98555500	1. 36119400	-4. 43509300
F	2. 02408300	1. 23469000	-3. 49622600
F	7. 66340400	-1. 43809200	-2. 82727300
F	6. 83401900	-3. 40228500	-2. 40632500
F	7. 54685400	-2. 15866400	-0. 77475300
S	4. 05188700	-3. 04162600	2. 25904000
C	-0. 12507000	-3. 33305600	5. 59339400
H	-0. 97774400	-3. 07238600	6. 23094400
H	-0. 33354300	-4. 30590300	5. 13405900
H	0. 75465800	-3. 44712300	6. 23849200
C	-1. 11949100	-2. 23431200	3. 58207400
H	-1. 20557300	-3. 17449600	3. 02695800
H	-2. 03883500	-2. 10308000	4. 16560000
H	-1. 08646800	-1. 41979700	2. 85239000
H	5. 22129200	-2. 33190900	0. 15844500
C	-0. 37800700	1. 21796600	4. 10562900
H	1. 73565200	-0. 96791100	0. 42303700
H	-1. 42560200	1. 02878700	4. 33189700
H	-0. 14630000	2. 17259800	3. 64086300
H	0. 80852500	-1. 54755900	2. 06405700
H	-1. 58498100	0. 96917100	2. 01152000
O	-0. 54919600	1. 51146900	-1. 04296700
O	-2. 40674500	-0. 31748600	-1. 03987700
P	-1. 21587500	0. 33180400	-0. 17208000
O	-0. 13308300	-0. 54960000	0. 32889600
C	-2. 91958900	4. 65156500	-2. 48666600
C	-2. 95258100	3. 40563800	-3. 10346600
C	-2. 08705900	2. 38225900	-2. 68942700
C	-1. 17615700	3. 85507900	-0. 96255000

C	-2.00464700	4.87673300	-1.45921300
C	-2.05157800	-0.97997000	-2.24734900
C	-1.80963000	-0.21284300	-3.38392900
C	-1.27418400	-0.84378600	-4.51906800
C	-1.08925700	-2.22149700	-4.54629600
C	-1.45915400	-2.97805000	-3.43588500
C	-1.93817600	-2.38221300	-2.25698700
H	-1.93089300	5.86088900	-1.00684000
H	-1.36318200	-4.05932600	-3.45866800
C	-2.12119800	1.24478900	-3.70269400
C	-3.57731200	1.40752900	-4.25342600
H	-3.69983000	0.95162500	-5.24079400
H	-4.27378700	0.91489100	-3.56536300
H	0.05161300	0.02051800	-6.00553900
H	-1.65895400	0.09206100	-6.43542300
C	-1.28963100	2.59136100	-1.56938400
H	-3.58084200	5.45054000	-2.81169200
H	-0.67441700	-2.70808300	-5.42501300
C	-3.82662000	2.93248200	-4.24479300
H	-3.52579900	3.39482000	-5.19494600
H	-4.88195500	3.18452700	-4.09226600
C	-0.95395600	0.16731200	-5.59618100
C	-1.08734600	1.51183300	-4.85055100
H	-1.39529100	2.33882400	-5.49694500
H	-0.12365200	1.77453300	-4.40624400
C	-2.36896100	-3.26836000	-1.12915200
C	-3.75345700	-3.48930700	-0.92304500
C	-1.40983100	-3.98402400	-0.37436200
C	-4.76848500	-2.88839200	-1.73534200
C	-4.18160600	-4.39699100	0.11705600
C	-1.85411600	-4.91635000	0.63857600
C	-6.09866400	-3.13471500	-1.51549900
H	-4.47199000	-2.23000500	-2.54440900
C	-5.58011000	-4.60887000	0.32796500
C	-3.22235400	-5.07865000	0.87108300
C	-6.51556700	-3.99656500	-0.46180000
H	-6.84626500	-2.66801000	-2.15127700
H	-5.88288500	-5.28409400	1.12483300
H	-3.55021700	-5.77427000	1.64107300
H	-7.57490500	-4.17326100	-0.29732000
C	-0.18670500	4.17461100	0.11420000
C	1.20122300	4.16303800	-0.18291900
C	-0.63911900	4.59885100	1.38906800
C	1.72786100	3.77881700	-1.45816100

C	2.14814100	4.58091700	0.82669700
C	0.32293700	5.01104600	2.38772200
C	3.07529800	3.78407000	-1.71025000
H	1.04447700	3.47854400	-2.24293500
C	3.54586500	4.58005500	0.52176100
C	1.68540000	4.98952900	2.08002600
C	4.00159800	4.18961200	-0.70842600
H	3.44140300	3.46915800	-2.68273100
H	4.23898000	4.90141300	1.29544200
H	2.40442300	5.29974500	2.83504000
H	5.06565700	4.19172500	-0.92772600
C	0.90116800	-4.59158900	0.13886900
H	1.96664500	-4.47044800	-0.03051600
C	0.00145200	-3.84673000	-0.57825200
H	0.35715900	-3.13729500	-1.31651900
C	0.45734400	-5.51740700	1.12652300
H	1.18979700	-6.09552300	1.68243300
C	-0.88122000	-5.66693600	1.37182100
H	-1.23399400	-6.36961000	2.12333000
C	-2.42553100	5.03917800	3.00007900
H	-3.48207500	5.03226300	3.25083100
C	-1.47415700	5.45367900	3.97417600
H	-1.81238100	5.77517200	4.95526000
C	-0.13911100	5.43587300	3.67309600
H	0.60092600	5.74220600	4.40844400
C	-2.02402700	4.62920300	1.75494800
H	-2.76650700	4.31146000	1.03233800
N	-2.09897800	0.96573900	1.12474700
S	-3.72254500	1.36739800	1.33278200
C	-4.62037300	-0.30006500	1.35827200
O	-4.21341900	2.08272900	0.16540000
O	-3.81377300	1.88228900	2.69301500
F	-5.09068500	-0.56990300	0.15062800
F	-3.78944100	-1.26290800	1.75844200
F	-5.62847800	-0.19252900	2.22101000

INT-4''

0 imaginary frequencies

H = -5198.729834

G = -5198.925503

E(M06-2X-DCM) = -5199.572203

O	1.92895800	-2.10241500	-0.00387400
O	3.66493500	-0.17635100	0.19236900
P	2.09523800	-0.52184500	0.15616300

O	1.63543000	-0.19594000	1.63835200
N	1.42332900	0.26850500	-1.02986800
S	-0.09946400	0.27705300	-1.54457700
C	-0.06762800	-0.96429800	-2.94586100
F	-1.31166600	-1.13465400	-3.39371400
F	0.42214900	-2.13305500	-2.52996400
F	0.69886500	-0.49948800	-3.93865300
C	-1.26288900	2.50900100	4.11186300
C	-0.03766200	3.44891600	3.85360300
H	0.75320100	3.13501900	4.54491000
H	-0.32644400	4.46010500	4.16869800
C	-0.13052200	4.32108900	1.41320100
C	-0.77158100	5.53648800	1.72065800
C	-0.14158700	3.89262900	0.07401300
C	-1.39411300	6.28996900	0.72658500
H	-0.76633100	5.91324100	2.73868600
C	-0.77853800	4.63749900	-0.91839300
H	0.33952700	2.96191700	-0.20285000
C	-1.40713800	5.84075100	-0.59562100
H	-1.87441100	7.22897700	0.98864800
H	-0.78140200	4.25835900	-1.93488800
H	-1.90855300	6.42151900	-1.36501700
C	0.56309800	3.51979800	2.46293700
C	-2.54568400	2.90400300	3.31541300
H	-3.42208000	2.60972600	3.89509500
H	-2.59101300	3.99271200	3.19044000
N	-2.72370900	2.27184100	2.01397600
C	-3.79944100	1.51176900	1.66569100
N	-3.68231400	1.00466700	0.38052300
C	-4.70277600	0.42559800	-0.39603100
C	-6.00088000	0.95771000	-0.42392900
C	-4.38860100	-0.65570900	-1.22985400
C	-6.96541400	0.39505100	-1.25508600
C	-5.36684200	-1.19902200	-2.06625000
H	-3.38336300	-1.06283600	-1.22912800
C	-6.66231300	-0.68701200	-2.08309000
H	-7.41427000	-1.10669900	-2.73998300
C	-5.04142800	-2.39841400	-2.91330600
C	-8.36903000	0.94092900	-1.23750000
F	-3.74854300	-2.41897000	-3.30270300
F	-5.26176200	-3.56166500	-2.23974400
F	-5.80192100	-2.45473200	-4.02829500
F	-8.97246200	0.80558300	-2.44158100
F	-9.14581500	0.29562700	-0.33793800

F	-8.39927300	2.25251600	-0.91591200
S	-5.10324300	1.19291600	2.68455000
H	-6.24859700	1.80982900	0.19343200
C	1.74339800	2.91929700	2.19880100
H	-2.73612400	0.79172900	0.06436200
H	2.29430100	2.40560800	2.98484500
H	2.25199300	3.04131500	1.24643000
O	-1.05549600	-0.25137400	-0.54724500
H	-2.11593500	2.57857800	1.26160200
O	-0.40638100	1.55426300	-2.18520800
H	1.46990500	0.76106200	1.81109000
C	5.72289600	-0.90330700	-3.38844300
C	5.44074900	-1.94602800	-2.51290700
C	4.84358400	-1.69217200	-1.26725000
C	4.73068800	0.69096700	-1.81705700
C	5.40395400	0.40218500	-3.01681600
C	2.54668000	-3.03026000	0.86718400
C	3.90173200	-3.30429700	0.70131000
C	4.53836100	-4.13089100	1.64214900
C	3.80825200	-4.75990900	2.64423300
C	2.43147700	-4.55583200	2.71222200
C	1.76429300	-3.67185500	1.84535100
H	5.65190000	1.22815900	-3.67615000
H	1.84496600	-5.07253900	3.46524400
C	4.88336000	-2.95856600	-0.41654900
C	4.86017300	-4.04609500	-1.54339100
H	3.82374600	-4.19817700	-1.86591500
H	5.24734600	-5.00997300	-1.20015000
H	6.30827600	-5.16956300	0.94237100
H	6.62030000	-4.07790600	2.28711100
C	4.42609200	-0.39625700	-0.97927900
H	6.19525400	-1.09642100	-4.34812800
H	4.29849300	-5.41469000	3.36010100
C	5.68181900	-3.42850800	-2.69565400
H	5.36070200	-3.78452600	-3.68091700
H	6.74894600	-3.67394700	-2.60502200
C	6.02540500	-4.19992500	1.37495400
C	6.23644600	-3.05021200	0.36848700
H	6.39518600	-2.10917300	0.90780600
H	7.09291400	-3.20226600	-0.29485900
C	0.28688300	-3.48896700	1.97364500
C	-0.26203300	-3.01270400	3.19170900
C	-0.56658400	-3.88361100	0.91206300
C	0.53695200	-2.60584200	4.31026200

C	-1.69798300	-2.92951600	3.33890700
C	-1.99640700	-3.72906300	1.05338500
C	-0.03484400	-2.22414800	5.49671800
H	1.61634700	-2.60225700	4.21225200
C	-2.25424800	-2.51671600	4.59051100
C	-2.52171000	-3.26116700	2.26039200
C	-1.45003800	-2.19117900	5.64905400
H	0.59929600	-1.93404700	6.33065300
H	-3.33663900	-2.46896700	4.67895600
H	-3.59971700	-3.16395600	2.36775800
H	-1.88444000	-1.88954300	6.59814200
C	4.41271300	2.11235400	-1.48007300
C	3.55033400	2.85905700	-2.32129800
C	5.05519800	2.73490200	-0.37964700
C	2.84553400	2.28164200	-3.42641000
C	3.34407900	4.26593400	-2.05998600
C	4.80896600	4.13437500	-0.11134100
C	2.04108400	3.04134900	-4.23396100
H	2.92660300	1.21634900	-3.60334500
C	2.50157000	5.02444600	-2.93182700
C	3.96847300	4.86007400	-0.96032300
C	1.87560100	4.43517000	-3.99647600
H	1.50462300	2.57060100	-5.05266300
H	2.36728100	6.08298200	-2.72328800
H	3.80023800	5.91667800	-0.76258000
H	1.23841500	5.02130500	-4.65305900
C	-0.94155700	-4.82236500	-1.31356500
H	-0.54564000	-5.26662400	-2.22301000
C	-0.08671300	-4.47234600	-0.30134400
H	0.97609800	-4.65338000	-0.41566300
C	-2.34295100	-4.60887200	-1.19302400
H	-3.00484400	-4.86107100	-2.01433100
C	-2.85193100	-4.08418600	-0.03591600
H	-3.92143400	-3.92717500	0.07244400
C	6.57394500	2.68733900	1.53758200
H	7.26903500	2.14194400	2.17044300
C	6.30272000	4.05735800	1.81419800
H	6.78373300	4.54272200	2.65889200
C	5.44808600	4.75714700	1.00662200
H	5.24079900	5.80773900	1.19558600
C	5.97559800	2.05254400	0.48048800
H	6.21064400	1.01324000	0.28079300
C	-1.61452500	2.68069000	5.60699000
H	-0.74370100	2.48402100	6.24353800

H	-1.96195200	3.69950400	5.82196000
H	-2.41021400	1.98673800	5.89848800
C	-0.89267600	1.04505500	3.84722500
H	-0.03419000	0.74210900	4.45771400
H	-1.72581600	0.38129000	4.09652600
H	-0.64666200	0.86481300	2.79718400

TS-EF-1S

1 imaginary frequencies

H = -5198.729113

G = -5198.921647

E(M06-2X-DCM) = -5199.563207

O	2.20192100	-2.02064900	-0.27462500
O	3.23761300	0.28281200	0.29518800
P	1.79967000	-0.46479600	0.06175100
O	1.03108200	-0.33342400	1.34066000
C	4.14770200	-4.16406700	2.75393400
C	4.86476000	-3.34387100	1.88934700
C	4.22217400	-2.68984900	0.82742200
C	2.08496500	-3.61962800	1.55186900
C	2.77576000	-4.31840900	2.55721300
C	4.18858100	0.31387400	-0.72464000
C	5.01096600	-0.79397500	-0.93156500
C	5.85739100	-0.81688100	-2.05181500
C	5.97054000	0.29300700	-2.88140400
C	5.22858100	1.43555800	-2.58582000
C	4.31483700	1.47087300	-1.51915600
H	2.20759000	-4.97562200	3.20899600
H	5.33197100	2.32227900	-3.20415900
C	5.25812400	-2.03876600	-0.08208800
C	6.41374300	-1.79661300	0.94786200
H	6.20599800	-0.87114700	1.49744000
H	7.38902300	-1.68537400	0.46392400
H	7.60353000	-2.09464600	-1.88830400
H	6.52058800	-2.54817900	-3.19987900
C	2.83634100	-2.77808500	0.70829300
H	4.64431500	-4.68322400	3.56994600
H	6.63198100	0.27849200	-3.74401700
C	6.33866300	-3.00166600	1.91045900
H	6.69987900	-2.76228900	2.91730600
H	6.94883700	-3.84145400	1.54920000
C	6.54449400	-2.15940200	-2.17541300
C	5.74509000	-3.03511600	-1.18730700
H	4.86751900	-3.45570100	-1.69142000

H	6. 32433400	-3. 86684700	-0. 77426000
C	3. 56157500	2. 73774000	-1. 26044800
C	2. 66070000	3. 23410200	-2. 23490400
C	3. 83699900	3. 49790000	-0. 09568300
C	2. 31013900	2. 49707900	-3. 41183000
C	2. 04605900	4. 52929400	-2. 04811500
C	3. 18453000	4. 77423400	0. 09594500
C	1. 45981400	3. 01702600	-4. 35123000
H	2. 69772800	1. 49413700	-3. 53503100
C	1. 17356700	5. 04133600	-3. 05954000
C	2. 31497400	5. 25724600	-0. 88620700
C	0. 89531700	4. 31364300	-4. 18490100
H	1. 19357400	2. 42350300	-5. 22091600
H	0. 73396100	6. 02473900	-2. 90938600
H	1. 84634900	6. 23005500	-0. 74878700
H	0. 23146000	4. 71331500	-4. 94714500
C	0. 60811000	-3. 81365100	1. 41490700
C	-0. 25126300	-3. 42127000	2. 47143700
C	0. 07944900	-4. 46544400	0. 27320500
C	0. 21447700	-2. 73306400	3. 63925300
C	-1. 66469400	-3. 71253600	2. 38903800
C	-1. 34161400	-4. 71518100	0. 18703100
C	-0. 63815000	-2. 40196200	4. 66107300
H	1. 26207100	-2. 46469400	3. 70216000
C	-2. 52089000	-3. 34323100	3. 47428400
C	-2. 17110500	-4. 34752500	1. 25105000
C	-2. 02615200	-2. 71365000	4. 58433100
H	-0. 25294700	-1. 89356600	5. 54174200
H	-3. 57996700	-3. 57737800	3. 39573100
H	-3. 23650000	-4. 55931800	1. 18915400
H	-2. 68726000	-2. 44245200	5. 40280600
C	5. 02367400	3. 84079600	2. 01685100
H	5. 74256300	3. 49679700	2. 75573200
C	4. 77230800	3. 07920700	0. 90516400
H	5. 29754800	2. 14099500	0. 76960600
C	4. 35814300	5. 08491900	2. 21226700
H	4. 57281300	5. 67855000	3. 09716400
C	3. 46729400	5. 53472200	1. 27456600
H	2. 96734300	6. 49304900	1. 39887500
C	0. 35059500	-5. 54076800	-1. 90368000
H	0. 99556000	-5. 87258600	-2. 71290800
C	-1. 05432500	-5. 74996800	-1. 99808900
H	-1. 46956100	-6. 22803100	-2. 88106100
C	-1. 87441800	-5. 35156800	-0. 97797100

H	-2.94946700	-5.49781300	-1.03784400
C	0.89635800	-4.92303300	-0.80936200
H	1.96867100	-4.77530200	-0.75619800
C	0.19539300	2.59315500	3.79263400
C	-0.21306700	3.62743200	2.69158900
H	0.24108900	4.59262100	2.97226600
H	0.29193500	3.35878200	1.76161500
C	-2.04096200	4.21418600	0.99346000
C	-1.45200700	3.52388500	-0.09011600
C	-3.07013100	5.14388700	0.71005200
C	-1.89993500	3.72264100	-1.39327500
H	-0.68070200	2.78051900	0.07793600
C	-3.49271300	5.36396900	-0.59476200
H	-3.50634100	5.72654500	1.51509900
C	-2.91761800	4.64464900	-1.64728500
H	-1.46091700	3.13487400	-2.19137200
H	-4.27247900	6.09382600	-0.79236900
H	-3.26369300	4.80274900	-2.66484700
C	-1.65485600	3.94273100	2.38200300
C	-0.72382400	1.33488700	3.81781700
H	-1.61276800	1.51041500	4.42282400
H	-0.16931700	0.51512400	4.28966600
N	-1.16167700	0.86763200	2.50324500
C	-2.42499600	0.61003700	2.13618100
N	-2.59609300	-0.05631400	0.97579100
C	-3.81273300	-0.27166800	0.26790500
C	-4.68334200	0.77569800	-0.04622600
C	-4.07372100	-1.55930300	-0.19922800
C	-5.83276300	0.51468900	-0.78909800
C	-5.22534600	-1.80575400	-0.94904100
H	-3.37154800	-2.35649700	0.01586000
C	-6.11587700	-0.77590900	-1.24232300
H	-7.00769300	-0.96966100	-1.82529100
C	-5.46932100	-3.20359800	-1.45456300
C	-6.79612000	1.63658400	-1.07342500
F	-4.59263500	-3.54956200	-2.42034700
F	-6.71047100	-3.35411900	-1.96109800
F	-5.32760700	-4.12058300	-0.46102700
F	-7.70880600	1.77440400	-0.08373000
F	-7.48477400	1.43087800	-2.21684200
F	-6.16192900	2.82591700	-1.18801500
S	-3.79663300	1.10874800	3.09160200
H	-4.45825000	1.78520500	0.27108400
H	-1.77577900	-0.45345900	0.49555000

H	-0.40251200	0.45284400	1.92870700
C	-2.65044200	3.92997000	3.36736700
H	-2.35533300	3.99386600	4.41108100
H	-3.10694500	2.68743600	3.28312000
H	-3.59813800	4.41750200	3.14000500
N	1.22118900	0.14521800	-1.31675100
S	-0.17426900	-0.25318000	-1.94928400
O	-0.84405700	0.90567500	-2.55434100
O	-1.00336800	-1.14471000	-1.09349100
C	0.28891700	-1.32329600	-3.40953800
F	1.04086600	-0.61920600	-4.26968800
F	-0.81926000	-1.72494800	-4.04030500
F	0.97945300	-2.39462300	-3.01326300
C	1.65037700	2.18028300	3.47536000
H	2.29606800	3.06192200	3.39635500
H	2.04633000	1.54504900	4.27669700
H	1.72515400	1.61595300	2.54241800
C	0.19013800	3.20170600	5.21204600
H	0.52031500	2.45423200	5.94317400
H	0.88698400	4.04549400	5.27038300
H	-0.79399200	3.55500500	5.53491800

TS-EF-1S-1

l imaginary frequencies

H= -5198.720562

G= -5198.909501

E(M06-2X-DCM) = -5199.563555

O	2.77240800	-0.37898700	0.16802600
O	1.21569400	-2.42949700	-0.24703900
P	1.18967600	-0.81095400	0.01273000
O	0.56480400	-0.46253800	1.33711000
C	5.26499200	-0.93112900	-3.15813800
C	4.89867100	-2.01097500	-2.36400200
C	4.16876500	-1.81626700	-1.18164000
C	4.09933800	0.57899800	-1.62584200
C	4.90870000	0.35251200	-2.75245800
C	1.77868700	-3.27901300	0.70548700
C	3.15266300	-3.50327600	0.67267400
C	3.74724100	-4.27675600	1.68186500
C	2.97125000	-4.88706400	2.66090600
C	1.58725800	-4.72176000	2.62537200
C	0.96159700	-3.91260200	1.66239200
H	5.23798300	1.21162500	-3.32899800
H	0.96362800	-5.21608700	3.36469900

C	4. 19287200	-3. 10662200	-0. 36587500
C	4. 29501500	-4. 16010300	-1. 51677000
H	4. 68608900	-5. 12224800	-1. 17030400
H	3. 29267500	-4. 32894700	-1. 92584900
H	5. 78369700	-4. 16485500	2. 46058900
H	5. 58327900	-5. 27018000	1. 10471100
C	3. 67574100	-0. 54455900	-0. 88687300
H	5. 83793600	-1. 07764900	-4. 07010500
H	3. 43022200	-5. 49182500	3. 43905800
C	5. 18544200	-3. 48117000	-2. 58081400
H	6. 24860100	-3. 71178000	-2. 42402700
H	4. 94057000	-3. 80251100	-3. 59944100
C	5. 24979600	-4. 30598600	1. 51371600
C	5. 49164600	-3. 15750700	0. 51326400
H	6. 39716300	-3. 28453100	-0. 08742000
H	5. 58318300	-2. 20981000	1. 05693000
C	-0. 53090700	-3. 80700900	1. 67219900
C	-1. 28444600	-4. 47522900	0. 67581000
C	-1. 18755700	-3. 13514700	2. 73135500
C	-0. 67792300	-5. 22533000	-0. 38168600
C	-2. 72854200	-4. 43903200	0. 72786900
C	-2. 63245900	-3. 12631100	2. 78512900
C	-1. 43573400	-5. 86668600	-1. 32566400
H	0. 40318000	-5. 28280400	-0. 43053400
C	-3. 48283700	-5. 10807600	-0. 28649100
C	-3. 36229200	-3. 76739000	1. 77891800
C	-2. 85708700	-5. 80289500	-1. 28537900
H	-0. 94820100	-6. 42572700	-2. 11957500
H	-4. 56628800	-5. 04279400	-0. 24819900
H	-4. 44925400	-3. 74661400	1. 81458800
H	-3. 44026800	-6. 30710400	-2. 05097700
C	3. 81207900	1. 99647600	-1. 23896600
C	4. 38196800	2. 52943700	-0. 05329000
C	3. 11129500	2. 84785400	-2. 13080700
C	5. 16918600	1. 74773700	0. 85342800
C	4. 22333800	3. 93540000	0. 24854100
C	2. 98572200	4. 25716700	-1. 82900600
C	5. 73485900	2. 29827700	1. 97423900
H	5. 33178400	0. 69937000	0. 63309000
C	4. 81725100	4. 46843800	1. 43659200
C	3. 53110500	4. 75829800	-0. 64436100
C	5. 55356400	3. 67801200	2. 27829900
H	6. 33476400	1. 67898800	2. 63581300
H	4. 68904300	5. 52916600	1. 64236500

H	3.43619500	5.82005000	-0.42371700
H	6.01397500	4.10000300	3.16796500
C	-1.14578100	-1.84149800	4.80492700
H	-0.58316100	-1.34811900	5.59395800
C	-0.47982500	-2.45365200	3.77477900
H	0.60241500	-2.42369300	3.73406300
C	-2.56981000	-1.84423000	4.85847000
H	-3.08016500	-1.35138900	5.68143700
C	-3.28746700	-2.46277600	3.87065700
H	-4.37463800	-2.46759700	3.89526300
C	1.87415600	3.22637900	-4.20307200
H	1.41354500	2.83008400	-5.10303000
C	1.78595500	4.61832700	-3.91799100
H	1.28410800	5.28093300	-4.61839200
C	2.31851200	5.11441000	-2.75872200
H	2.24573000	6.17325700	-2.52094300
C	2.51257100	2.37166200	-3.34217700
H	2.54873800	1.31298000	-3.56888100
N	0.44076300	-0.14333500	-1.22912600
S	0.30455200	-0.51319400	-2.77619300
C	-0.85007500	-2.00181000	-2.82635500
O	1.53780100	-0.99556500	-3.41805300
O	-0.46290400	0.55276600	-3.43596600
F	-0.15958900	-3.13747800	-2.69669700
F	-1.76142600	-1.93548300	-1.84137500
F	-1.48987000	-2.01977500	-3.99988900
C	1.00919500	2.84211300	3.90795000
C	0.88724800	3.74992500	2.63419300
H	1.55264900	4.61454600	2.78785600
H	1.33024700	3.22203600	1.78831000
C	-0.75896500	4.37124000	0.76415300
C	-0.35918300	3.33662900	-0.11282700
C	-1.55983900	5.41406400	0.24037600
C	-0.78101400	3.31739800	-1.43958300
H	0.22464200	2.49746600	0.24773200
C	-1.95501200	5.40871100	-1.09167900
H	-1.83861500	6.25014500	0.87412500
C	-1.57775300	4.35462600	-1.93025300
H	-0.50226800	2.48483400	-2.07843300
H	-2.56187400	6.22320400	-1.47635900
H	-1.90987300	4.33624300	-2.96358700
C	-0.43794300	4.33019000	2.19617900
C	-0.23821900	1.94207000	4.12779400
H	-1.05079500	2.48573400	4.60746400

H	0.04205600	1.12352700	4.80341500
N	-0.74022100	1.35914700	2.89216000
C	-1.99459000	1.37090800	2.43189000
N	-2.22898400	0.58566200	1.35720800
C	-3.33458100	0.63111300	0.46124100
C	-3.82856900	1.84263800	-0.03539800
C	-3.87335000	-0.57508100	0.01597800
C	-4.87749400	1.83526900	-0.95012200
C	-4.91866700	-0.56693500	-0.91161500
H	-3.48022300	-1.51381000	0.39106400
C	-5.43271900	0.63273200	-1.39396600
H	-6.24979900	0.63385400	-2.10447000
C	-5.47585300	-1.88597700	-1.38073300
C	-5.36132300	3.13848500	-1.53064600
F	-4.55666000	-2.60239200	-2.05688300
F	-6.54646100	-1.73020900	-2.18656900
F	-5.87435100	-2.65263300	-0.33127500
F	-5.21352600	4.16392800	-0.66254800
F	-6.66629700	3.07950000	-1.87369000
F	-4.67591400	3.47208700	-2.65000400
S	-3.24948900	2.33390400	3.16472100
H	-3.39547200	2.78055800	0.28276900
H	-1.44788500	-0.02551900	1.09051300
H	-0.09046600	0.74022500	2.37567500
C	-1.39521100	4.76759800	3.11241600
H	-1.10378900	4.93980400	4.14515500
H	-2.20755200	3.65557600	3.20126600
H	-2.19632100	5.41374100	2.75503800
C	2.25205700	1.94932300	3.69361700
H	3.13793900	2.55930900	3.48994900
H	2.45301300	1.35228200	4.59144000
H	2.12759800	1.26060500	2.85078100
C	1.22945400	3.66439400	5.19457700
H	1.32144500	3.00048900	6.06256800
H	2.15683000	4.24369800	5.12502400
H	0.41239600	4.36283600	5.40292800

TS-EF-1S-2

1 imaginary frequencies

H = -5198.726621

G = -5198.918062

E(M06-2X-DCM) = -5199.560199

0	1.98619700	-2.31294300	-0.31419600
0	3.16569000	-0.04724900	0.13369600

P	1. 69552900	-0. 70116900	-0. 20037000
O	0. 80066100	-0. 35810700	0. 94950700
C	3. 78258500	-4. 33907000	2. 88459900
C	4. 55400500	-3. 66162000	1. 94654300
C	3. 95481500	-3. 03261000	0. 84454800
C	1. 75833300	-3. 71470500	1. 65876300
C	2. 39918800	-4. 38205500	2. 71643900
C	4. 18161800	-0. 10752000	-0. 82172100
C	4. 88631300	-1. 29653100	-1. 00485300
C	5. 73792300	-1. 42332800	-2. 11323600
C	5. 98949400	-0. 33519100	-2. 94185100
C	5. 40322700	0. 89382500	-2. 63863500
C	4. 48645200	1. 03758800	-1. 58399700
H	1. 78513100	-4. 93116000	3. 42443500
H	5. 63888300	1. 76812300	-3. 23828300
C	5. 02517700	-2. 53013900	-0. 11710200
C	6. 22207300	-2. 34173700	0. 87959100
H	6. 11605800	-1. 36872900	1. 37352900
H	7. 19239000	-2. 35413600	0. 37397000
H	7. 33794100	-2. 88180800	-1. 94883700
H	6. 18452800	-3. 24318900	-3. 22789300
C	2. 56478000	-3. 01040000	0. 74208500
H	4. 24618300	-4. 83540100	3. 73353200
H	6. 65082200	-0. 42827300	-3. 79959800
C	6. 05395200	-3. 46967600	1. 91829000
H	6. 46474100	-3. 20732800	2. 90009000
H	6. 56564600	-4. 38837400	1. 59820500
C	6. 27227100	-2. 83673300	-2. 21378000
C	5. 40271900	-3. 60283600	-1. 19076900
H	4. 48418900	-3. 95538800	-1. 67333500
H	5. 90778000	-4. 47100200	-0. 75526600
C	3. 95992000	2. 40282000	-1. 26365600
C	3. 13679800	3. 09258300	-2. 18744100
C	4. 40532200	3. 05634500	-0. 08541200
C	2. 64052800	2. 48270200	-3. 38345000
C	2. 76520600	4. 46735400	-1. 93010500
C	4. 00127600	4. 42101500	0. 17264500
C	1. 87480400	3. 18680500	-4. 27562100
H	2. 84407900	1. 43434000	-3. 56052600
C	1. 97004600	5. 16745400	-2. 89009000
C	3. 19668500	5. 08813000	-0. 75515000
C	1. 54617800	4. 55090800	-4. 03661600
H	1. 48891400	2. 68661300	-5. 15800700
H	1. 71095600	6. 20389100	-2. 68607300

H	2.91549300	6.12291600	-0.56742400
H	0.94453800	5.09411000	-4.76085600
C	0.27074900	-3.81279900	1.53448400
C	-0.56170800	-3.22058700	2.51531400
C	-0.29835600	-4.56964600	0.48159100
C	-0.04768600	-2.45136100	3.60956100
C	-1.99531600	-3.38532400	2.42977200
C	-1.73483800	-4.70243100	0.39194500
C	-0.87914300	-1.92285000	4.56329800
H	1.02187200	-2.29021100	3.67510800
C	-2.82798700	-2.80293300	3.43696900
C	-2.54327000	-4.11004000	1.36695100
C	-2.29060700	-2.09892600	4.48070000
H	-0.45946700	-1.36151200	5.39459200
H	-3.90377500	-2.94024800	3.35662600
H	-3.62351600	-4.21207600	1.29251000
H	-2.93415000	-1.66889800	5.24308000
C	5.71120400	3.10484300	1.98497300
H	6.38234700	2.61049900	2.68230600
C	5.28488200	2.44120600	0.86380800
H	5.62746700	1.42976400	0.67930400
C	5.29094100	4.44059100	2.24409300
H	5.64165200	4.95365300	3.13579500
C	4.46117600	5.07572500	1.35909200
H	4.14747600	6.10308400	1.53218200
C	-0.09173000	-5.94038300	-1.52991000
H	0.53223900	-6.42987800	-2.27286700
C	-1.50854500	-6.04188600	-1.62930500
H	-1.95190600	-6.59864400	-2.45035100
C	-2.30459700	-5.44198300	-0.69196100
H	-3.38696200	-5.50446500	-0.75789900
C	0.49096200	-5.23140900	-0.51270400
H	1.57130600	-5.16746400	-0.45239300
C	0.59926500	2.84262500	3.40663400
C	0.22073900	3.86267700	2.28420500
H	0.76999600	4.79580000	2.49244200
H	0.64375600	3.51151900	1.34082200
C	-1.61866800	4.53886400	0.64465200
C	-1.17212300	3.71991600	-0.41463300
C	-2.50643300	5.59703400	0.34409700
C	-1.61499900	3.93241600	-1.71709200
H	-0.53143000	2.86689100	-0.22619300
C	-2.91977000	5.82740700	-0.96292300
H	-2.83209600	6.26742900	1.13360000

C	-2.48141600	4.99132200	-1.99503800
H	-1.28437400	3.25883800	-2.50074300
H	-3.58406700	6.65942000	-1.17870000
H	-2.81782400	5.16495500	-3.01340300
C	-1.20704800	4.28659400	2.03335200
C	-0.44583300	1.70134300	3.55586400
H	-1.26806100	2.00113400	4.20394000
H	0.04332900	0.84395200	4.03309000
N	-1.01307600	1.23419500	2.29255700
C	-2.31528100	1.07329100	2.02230500
N	-2.60567300	0.41989800	0.88147600
C	-3.86207900	0.13590100	0.27993700
C	-4.90679100	1.06257600	0.19752100
C	-3.99477400	-1.11542200	-0.32727800
C	-6.09015400	0.70770400	-0.44764800
C	-5.18196200	-1.45127000	-0.97929800
H	-3.17206000	-1.82046600	-0.29166000
C	-6.24174900	-0.54972500	-1.03498500
H	-7.16584800	-0.81640600	-1.53294200
C	-5.31136600	-2.82624200	-1.58140600
C	-7.19352600	1.72474300	-0.58514800
F	-4.21613700	-3.16677700	-2.28853800
F	-6.37907800	-2.92604500	-2.39874700
F	-5.46282300	-3.77579500	-0.61756300
F	-7.17501100	2.62821000	0.41875100
F	-8.41181300	1.14061700	-0.58658500
F	-7.08914400	2.41849300	-1.74191500
S	-3.55671400	1.71019300	3.07464500
H	-4.80077200	2.04706600	0.62989900
H	-1.80877400	0.15121800	0.28967400
H	-0.34574400	0.72115700	1.68575100
C	-2.14683400	4.42457200	3.05517000
H	-1.80421000	4.50470200	4.08359200
H	-2.74893600	3.19145300	3.08499800
H	-3.06181800	4.97487400	2.83685100
N	1.34634200	-0.30294400	-1.72476200
S	-0.08086500	-0.03300500	-2.33988800
O	0.01879400	0.57284100	-3.66847000
O	-1.05673300	0.58089100	-1.39622300
C	-0.82443700	-1.72130300	-2.64332400
F	-0.03453000	-2.46835300	-3.41279500
F	-2.01921600	-1.59418800	-3.23224700
F	-0.99885500	-2.34625600	-1.46213700
C	1.96959200	2.24691200	3.01581100

H	2.70851100	3.03905000	2.85644300
H	2.34308900	1.59851200	3.81738500
H	1.91398100	1.64478300	2.10449200
C	0.75795400	3.51631000	4.78640700
H	1.03591600	2.77243400	5.54263800
H	1.55613100	4.26649100	4.75679000
H	-0.15456900	4.00969500	5.13641200

TS-EF-1S-3

l imaginary frequencies

H = -5198.729379

G = -5198.920227

E(M06-2X-DCM) = -5199.561272

O	1.40983300	-2.56809400	-0.49846400
O	3.09534000	-0.74792800	0.25759700
P	1.53678300	-0.95757800	-0.21467600
O	0.67572600	-0.50229700	0.92020700
C	2.37902600	-5.29347000	2.53326000
C	3.36668500	-4.75840900	1.71342200
C	3.03324000	-3.89024100	0.66291000
C	0.68015300	-4.03666000	1.29577200
C	1.04874600	-4.94949100	2.29982300
C	4.12894500	-0.98108700	-0.65126700
C	4.51768600	-2.29019100	-0.93184300
C	5.38981300	-2.52927400	-2.00515600
C	5.97331000	-1.47101200	-2.69336900
C	5.69686900	-0.16590000	-2.28566000
C	4.76843900	0.11203600	-1.26851000
H	0.26386800	-5.38002600	2.91472200
H	6.19083300	0.66906700	-2.77378400
C	4.26646800	-3.59683700	-0.18406800
C	5.39289100	-3.82863300	0.88315100
H	5.50294400	-2.91533900	1.47956500
H	6.36290700	-4.04626600	0.42600800
H	6.54412100	-4.36677000	-1.92844600
H	5.43894800	-4.28593100	-3.29557900
C	1.70725300	-3.49098300	0.50015500
H	2.63403000	-5.97478900	3.34117100
H	6.65274300	-1.65188200	-3.52246800
C	4.86292700	-4.96847700	1.77686700
H	5.25289700	-4.92200300	2.80021400
H	5.14286300	-5.95365100	1.37763700
C	5.54956100	-4.01694000	-2.23882900
C	4.43614100	-4.62162300	-1.35325900

H	3. 49774700	-4. 67037900	-1. 91710900
H	4. 66552300	-5. 63047900	-0. 99550500
C	4. 57334200	1. 53209300	-0. 83415500
C	4. 03630800	2. 48964800	-1. 72987500
C	5. 05723000	1. 94236700	0. 43522900
C	3. 51087600	2. 13626300	-3. 01366800
C	4. 00028500	3. 88581000	-1. 35106000
C	4. 98811100	3. 33742700	0. 81098900
C	3. 02927000	3. 08964000	-3. 87235900
H	3. 45918200	1. 09070700	-3. 28928800
C	3. 49606200	4. 84908800	-2. 27951100
C	4. 46625000	4. 26874900	-0. 09083200
C	3. 03475100	4. 46615000	-3. 51034100
H	2. 61072700	2. 78544400	-4. 82637100
H	3. 48915900	5. 89538600	-1. 98257500
H	4. 43934600	5. 32072800	0. 18796800
H	2. 65690800	5. 20788600	-4. 20936500
C	-0. 77237100	-3. 72965600	1. 10888800
C	-1. 49499900	-3. 09432500	2. 14911100
C	-1. 44788500	-4. 17181900	-0. 05528900
C	-0. 86842600	-2. 59002000	3. 33550500
C	-2. 92643100	-2. 93235900	2. 03141200
C	-2. 87286700	-3. 96093700	-0. 17796800
C	-1. 60158000	-2. 01817900	4. 34367200
H	0. 20915200	-2. 66141400	3. 42497400
C	-3. 65618400	-2. 33875900	3. 11067300
C	-3. 57520200	-3. 35955300	0. 86976900
C	-3. 01743400	-1. 89753900	4. 23867500
H	-1. 09972700	-1. 65582400	5. 23761000
H	-4. 73561200	-2. 25311100	3. 01161400
H	-4. 64925300	-3. 21387900	0. 77848000
H	-3. 58339400	-1. 45305200	5. 05279200
C	6. 13264800	1. 46966900	2. 58320400
H	6. 58807200	0. 75894400	3. 26768200
C	5. 66008100	1. 03968800	1. 37044100
H	5. 75200600	-0. 00620800	1. 10217000
C	6. 04200700	2. 84126300	2. 95506400
H	6. 42594100	3. 16599400	3. 91863800
C	5. 48658800	3. 74482300	2. 08902400
H	5. 42805600	4. 79952900	2. 34977500
C	-1. 46294000	-5. 23749300	-2. 25446100
H	-0. 93031800	-5. 73712100	-3. 05911700
C	-2. 86166700	-5. 00312800	-2. 38077600
H	-3. 38200300	-5. 32004500	-3. 28048600

C	-3.54362600	-4.38828700	-1.36636400
H	-4.61405300	-4.21277100	-1.44293000
C	-0.78406500	-4.84283900	-1.13174100
H	0.27892900	-5.03783400	-1.05263600
C	0.95107300	2.52528900	3.61635700
C	0.90323400	3.65574700	2.54067700
H	1.64858800	4.41538100	2.83102800
H	1.29172900	3.25646300	1.60100000
C	-0.53790500	4.93024300	0.86781000
C	-0.17551600	4.15073600	-0.25126500
C	-1.11401200	6.20141300	0.64167300
C	-0.40244200	4.61245100	-1.54468000
H	0.21645600	3.14832900	-0.12971200
C	-1.30643000	6.67306700	-0.65120000
H	-1.36461600	6.83689100	1.48553200
C	-0.95819500	5.87685100	-1.74749300
H	-0.14831900	3.97176700	-2.38265600
H	-1.72795700	7.66216200	-0.80644400
H	-1.12339300	6.24244000	-2.75722700
C	-0.35422800	4.43341300	2.23732700
C	-0.32888400	1.64493600	3.62121100
H	-1.12495100	2.10269700	4.20671100
H	-0.08648800	0.68965300	4.10354400
N	-0.86285500	1.33920200	2.29570600
C	-2.13865800	1.46548100	1.91075500
N	-2.44916400	0.93525700	0.70857500
C	-3.73111400	0.80437200	0.12294200
C	-3.88078600	1.11177200	-1.23381700
C	-4.80938600	0.29039300	0.84541500
C	-5.11228800	0.90721100	-1.85400700
C	-6.03747000	0.10068400	0.21179600
H	-4.68078000	0.00751700	1.88292000
C	-6.20071300	0.40610400	-1.13828600
H	-7.15557900	0.25349000	-1.62519200
C	-7.16080200	-0.50107400	1.01212900
C	-5.24158100	1.17885400	-3.33131600
F	-6.85889400	-1.77001700	1.40503500
F	-8.31269400	-0.56656600	0.31709300
F	-7.40143900	0.19734500	2.14197400
F	-4.52154000	2.25751300	-3.70458900
F	-6.52668800	1.40289000	-3.68779000
F	-4.80237600	0.13428900	-4.06635800
S	-3.31459500	2.35383200	2.84807900
H	-3.03467500	1.49832900	-1.79018400

H	-1.66463700	0.70394500	0.08496000
H	-0.27174100	0.71204000	1.71930100
C	-1.35098200	4.67519100	3.18713400
H	-1.10813300	4.58035700	4.24256200
H	-2.18280300	3.62625900	3.03514200
H	-2.08887400	5.44478600	2.96090400
N	1.41683000	-0.34479900	-1.70375100
S	0.17673800	0.36613200	-2.36033800
O	0.52810000	0.98042800	-3.64087500
O	-0.62680100	1.20278900	-1.41694400
C	-1.03264900	-0.99410200	-2.79641400
F	-0.44888200	-1.94970600	-3.51685300
F	-2.05549800	-0.48089000	-3.49498500
F	-1.52081900	-1.53215700	-1.66471000
C	2.17947600	1.65061500	3.28003300
H	3.08861200	2.25828200	3.22203600
H	2.33224100	0.89642500	4.06118700
H	2.06270200	1.12166400	2.32964700
C	1.14759700	3.07882900	5.04390900
H	1.18821400	2.25658900	5.76825000
H	2.09521700	3.62444200	5.11526900
H	0.34707100	3.75392700	5.36306500

TS-EF-1S-4

1 imaginary frequencies

H = -5198.723515

G = -5198.913607

E(M06-2X-DCM) = -5199.557805

O	-1.94142700	2.30568100	-0.27055500
O	-3.18815700	0.07869200	0.19682300
P	-1.69754900	0.68436900	-0.14679400
O	-0.81520200	0.33241500	1.01073600
C	-3.59141000	4.37701100	2.97902300
C	-4.40671600	3.72347600	2.06137400
C	-3.85520900	3.08359300	0.94111800
C	-1.62029000	3.70781200	1.69090400
C	-2.21315900	4.38738300	2.76875700
C	-4.21192000	0.18324900	-0.74479600
C	-4.88351000	1.39568600	-0.90047900
C	-5.75208000	1.56387700	-1.98998500
C	-6.05115600	0.49654000	-2.82953700
C	-5.49492700	-0.75258100	-2.55566100
C	-4.56437100	-0.93991800	-1.51952200
H	-1.56506500	4.92047400	3.45841900

H	-5.76686000	-1.61020900	-3.16386100
C	-4.96453400	2.62156900	0.00453400
C	-6.14020700	2.45910000	1.03006300
H	-6.05038000	1.47888100	1.51286000
H	-7.12256100	2.50479900	0.55012100
H	-7.30604000	3.06328500	-1.76939600
H	-6.17250900	3.41073500	-3.07004300
C	-2.46983800	3.02317100	0.79842800
H	-4.01698200	4.88161900	3.84287200
H	-6.72585500	0.62150800	-3.67268300
C	-5.91170700	3.57240700	2.07338500
H	-6.30207200	3.31209600	3.06405600
H	-6.40684400	4.50764000	1.77596400
C	-6.24834900	2.99265900	-2.05969200
C	-5.33470700	3.71895200	-1.04686300
H	-4.41707500	4.05089200	-1.54551900
H	-5.80383900	4.59564700	-0.58889400
C	-4.08127700	-2.32915000	-1.23703100
C	-3.32769000	-3.03617200	-2.20620900
C	-4.51555400	-2.98901700	-0.05782600
C	-2.83397900	-2.41824200	-3.39934000
C	-3.03128900	-4.43789100	-2.00262000
C	-4.17599900	-4.37937300	0.15129700
C	-2.14973500	-3.13820800	-4.34301600
H	-2.97130900	-1.35272500	-3.53154900
C	-2.32686900	-5.15691600	-3.01942800
C	-3.45121600	-5.06647900	-0.82690500
C	-1.90975200	-4.52988400	-4.16404900
H	-1.76082400	-2.63375600	-5.22156300
H	-2.13805400	-6.21699800	-2.86394300
H	-3.23078700	-6.12261500	-0.68071000
H	-1.38309100	-5.08840800	-4.93392400
C	-0.13606200	3.78034800	1.51912600
C	0.71795400	3.17626400	2.47365000
C	0.41079500	4.53144600	0.45025300
C	0.22680900	2.41155400	3.58155600
C	2.15027500	3.32421900	2.34614800
C	1.84551200	4.64456800	0.31659400
C	1.07925800	1.87288600	4.51062000
H	-0.84212900	2.26106600	3.67588900
C	3.00484300	2.73302400	3.32960500
C	2.67524100	4.04185500	1.26706000
C	2.48960900	2.03490600	4.38847700
H	0.67784800	1.31350900	5.35213800

H	4. 07934400	2. 85914100	3. 21899900
H	3. 75399200	4. 13032800	1. 16006100
H	3. 14964300	1. 59826800	5. 13275100
C	-5. 74345500	-3. 02322000	2. 05977000
H	-6. 36083100	-2. 51287800	2. 79421200
C	-5. 32593300	-2. 35409400	0. 93859700
H	-5. 62190500	-1. 32219400	0. 79148200
C	-5. 38394800	-4. 38471200	2. 27106800
H	-5. 72628100	-4. 90132000	3. 16394000
C	-4. 62360400	-5. 03948900	1. 33934700
H	-4. 35809500	-6. 08569500	1. 47595800
C	0. 16160200	5. 91099400	-1. 55042000
H	-0. 47807200	6. 41186800	-2. 27215000
C	1. 57588400	5. 99152700	-1. 69431400
H	2. 00147800	6. 54358800	-2. 52785200
C	2. 39189500	5. 37750300	-0. 78371000
H	3. 47250500	5. 42379400	-0. 88362400
C	-0. 39933100	5. 20729100	-0. 51747100
H	-1. 47806100	5. 15879300	-0. 42373200
C	-0. 60295800	-2. 90129600	3. 38123900
C	-0. 20006500	-3. 87808800	2. 22470500
H	-0. 77257300	-4. 80727900	2. 37308500
H	-0. 58444100	-3. 44021400	1. 30333100
C	1. 72382800	-4. 42002000	0. 61177900
C	0. 83393100	-4. 50253600	-0. 48248400
C	3. 11114200	-4. 44083300	0. 32887800
C	1. 30679100	-4. 58996800	-1. 78810300
H	-0. 23849900	-4. 51167700	-0. 32662700
C	3. 58144400	-4. 50651400	-0. 97658900
H	3. 83199600	-4. 36359600	1. 13505500
C	2. 67887800	-4. 58031500	-2. 04139900
H	0. 59503000	-4. 64016800	-2. 60554800
H	4. 65037100	-4. 46882900	-1. 16440400
H	3. 04434700	-4. 61854800	-3. 06348800
C	1. 24479100	-4. 27531400	1. 99419700
C	0. 42176100	-1. 74415500	3. 56130000
H	1. 23504100	-2. 03379900	4. 22491800
H	-0. 09027900	-0. 89577500	4. 03039900
N	1. 00434800	-1. 26402100	2. 30986100
C	2. 30443200	-1. 10129300	2. 04616800
N	2. 60271800	-0. 45387300	0. 90443000
C	3. 85447600	-0. 19512600	0. 28508400
C	4. 90691300	-1. 11235300	0. 24943000
C	3. 97421000	1. 01955800	-0. 39939000

C	6.07755100	-0.79684500	-0.44030600
C	5.15229500	1.32219700	-1.08073100
H	3.14621200	1.71901100	-0.40180900
C	6.21618100	0.42052000	-1.10445500
H	7.12798400	0.65741200	-1.63776300
C	5.27756200	2.66584000	-1.75144100
C	7.16138600	-1.83959400	-0.50885000
F	4.15290700	3.00675100	-2.40830000
F	6.29873100	2.70060000	-2.63192800
F	5.51117900	3.65035000	-0.84011600
F	7.40252000	-2.38840400	0.70252100
F	8.32436300	-1.34161200	-0.97221200
F	6.81146900	-2.86430900	-1.33023800
S	3.53930700	-1.72446800	3.12369800
H	4.81398900	-2.06778700	0.74338900
H	1.80598200	-0.20079100	0.30251600
H	0.33626300	-0.76644000	1.68897800
C	2.12732200	-4.43700200	3.06113800
H	1.72080200	-4.50172300	4.06471900
H	2.76419200	-3.18429400	3.13377700
H	3.02688900	-5.03026600	2.91287400
N	-1.36949000	0.25171500	-1.66297800
S	0.04867700	-0.02767800	-2.30246300
O	-0.08393300	-0.68405000	-3.60294400
O	1.05686200	-0.58152600	-1.36069400
C	0.74776300	1.65964100	-2.69747000
F	-0.08702900	2.36781600	-3.45769000
F	1.91749200	1.53026000	-3.33534800
F	0.96440500	2.33152700	-1.54936900
C	-1.97870600	-2.31653900	2.98967300
H	-2.70234500	-3.11565400	2.79809100
H	-2.37344300	-1.69873600	3.80499500
H	-1.92121400	-1.68617500	2.09795900
C	-0.77597500	-3.60609600	4.74373900
H	-1.10190300	-2.88425700	5.50221300
H	-1.54845000	-4.38043900	4.67745600
H	0.13868600	-4.07591100	5.11782400

TS-EF-1R

1 imaginary frequencies

H = -5198.724770

G = -5198.916070

E(M06-2X-DCM) = 5199.561361

O	-3.19743700	0.11786600	-0.92546200
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O	-2.11681500	-1.73780200	0.53521200
P	-1.74729100	-0.43113300	-0.39084400
O	-1.04271900	0.52068300	0.53489600
C	-6.27916900	1.11947100	1.72720500
C	-6.03627600	-0.20833900	1.39257600
C	-5.05274400	-0.54341500	0.44838200
C	-4.49153000	1.82172100	0.20974400
C	-5.53285800	2.11953200	1.10601100
C	-2.65888500	-2.88161500	-0.04992400
C	-4.01511700	-2.91171700	-0.36362300
C	-4.51394100	-3.97172300	-1.13639700
C	-3.69954300	-5.04808000	-1.47211800
C	-2.38209200	-5.06932000	-1.01262200
C	-1.82895800	-3.99092100	-0.30299200
H	-5.74466000	3.16297100	1.31996100
H	-1.75039200	-5.92801600	-1.22027700
C	-5.16831100	-2.02300700	0.08997800
C	-5.79250400	-2.57744500	1.41679900
H	-4.98623400	-2.73892200	2.14199700
H	-6.30432600	-3.53332700	1.27001100
H	-6.63386500	-4.39507100	-0.93372800
H	-6.16586900	-3.90585200	-2.55825200
C	-4.23487700	0.46259100	-0.06795900
H	-7.05191000	1.38018000	2.44616400
H	-4.08339500	-5.87294700	-2.06703800
C	-6.72200000	-1.45151900	1.91470400
H	-6.83305900	-1.44397000	3.00527500
H	-7.73354000	-1.55245000	1.49692100
C	-5.96448700	-3.72860700	-1.49561300
C	-6.16976000	-2.25092300	-1.09172300
H	-5.88551100	-1.59639900	-1.92351100
H	-7.20268500	-2.01471400	-0.81718200
C	-0.42892600	-4.09034500	0.21734100
C	0.66737700	-4.16394100	-0.67652600
C	-0.21498400	-4.21449900	1.61455900
C	0.51999300	-4.01792200	-2.09339300
C	2.00211800	-4.37352600	-0.15768400
C	1.12761600	-4.39752100	2.11979500
C	1.59941400	-4.10051000	-2.93355100
H	-0.45830400	-3.79223800	-2.49858600
C	3.10010500	-4.46237900	-1.07068600
C	2.19660400	-4.47444300	1.22226500
C	2.90641400	-4.33675300	-2.42120600
H	1.46007200	-3.94637300	-3.99852800

H	4.09804900	-4.61727700	-0.66750200
H	3.20297600	-4.62569500	1.60760400
H	3.75237500	-4.38343100	-3.10021700
C	-3.75554000	2.94554500	-0.44861500
C	-3.02411200	3.87121400	0.33680000
C	-3.87823200	3.14502100	-1.84760600
C	-2.86789600	3.73928400	1.75543500
C	-2.40393100	5.01467600	-0.29497600
C	-3.22046900	4.27182500	-2.46953400
C	-2.20029400	4.68321400	2.49343600
H	-3.29489400	2.87383000	2.24855800
C	-1.70694600	5.96938700	0.51073400
C	-2.50582400	5.17483000	-1.67867900
C	-1.61495200	5.82023200	1.86757300
H	-2.11447600	4.56360000	3.57060400
H	-1.25544500	6.82575500	0.01520200
H	-2.02976800	6.03214900	-2.15063200
H	-1.09083400	6.55821600	2.46872200
C	-1.04220600	-4.33477500	3.91638300
H	-1.87513400	-4.33369100	4.61497100
C	-1.28149300	-4.20195900	2.57205000
H	-2.30088000	-4.10142900	2.21757800
C	0.28560700	-4.49085900	4.40787700
H	0.45758800	-4.59724800	5.47573200
C	1.33565800	-4.52214300	3.52990900
H	2.35428000	-4.65231500	3.88764700
C	-4.74923300	2.50794400	-4.04112200
H	-5.34572100	1.83902700	-4.65542900
C	-4.06947700	3.59901700	-4.65192300
H	-4.14615500	3.74918300	-5.72527900
C	-3.33278800	4.45781100	-3.88283100
H	-2.81954400	5.30496100	-4.33180400
C	-4.65859900	2.29143000	-2.69136400
H	-5.19115700	1.45864800	-2.24801000
N	-1.08551200	-0.96493000	-1.75348100
S	0.08384600	-0.32755200	-2.60322500
O	0.36770200	-1.14358900	-3.78238200
O	1.24248100	0.14168400	-1.79602400
C	-0.58536700	1.28095300	-3.28660800
F	-1.71524500	1.07398200	-3.96298400
F	0.31723500	1.83881500	-4.10060000
F	-0.83676100	2.13964100	-2.27875700
C	-0.28425100	0.43641700	4.23068600
C	0.08540000	1.91212100	3.84739400

H	-0.26796400	2.55241800	4.67125700
H	-0.51909700	2.20051300	2.98757800
C	1.82850100	3.14009200	2.40793100
C	1.08706000	3.01340600	1.21116800
C	2.92252500	4.03740200	2.41804200
C	1.45601200	3.71375400	0.06619500
H	0.25287200	2.32544100	1.13691600
C	3.27226200	4.75356800	1.27874200
H	3.47921900	4.20285200	3.33481000
C	2.54707700	4.58432000	0.09493000
H	0.89203300	3.55713900	-0.84761200
H	4.11310000	5.43996300	1.31144400
H	2.83282200	5.13075500	-0.79954000
C	1.51690900	2.32585400	3.59341400
C	0.58828400	-0.63063600	3.49660500
H	1.43572300	-0.92451200	4.11431700
H	-0.02187800	-1.52705200	3.33927500
N	1.12111000	-0.22187200	2.19608300
C	2.40379400	-0.30253000	1.81589300
N	2.67463900	-0.20229400	0.50437000
C	3.96602900	-0.05355500	-0.08538500
C	4.77596700	1.04544400	0.21187500
C	4.37132600	-0.98719500	-1.03687200
C	6.00931000	1.18188900	-0.42160400
C	5.61031700	-0.83824300	-1.66579100
H	3.72448900	-1.82236500	-1.28260200
C	6.43723700	0.23958300	-1.36021100
H	7.39397100	0.35370100	-1.85429100
C	6.03772800	-1.88227500	-2.66519200
C	6.90073900	2.33897400	-0.05589600
F	5.14454700	-2.00915600	-3.66839200
F	7.23573600	-1.60002000	-3.21799200
F	6.14240700	-3.10384200	-2.08351900
F	7.64834800	2.06786700	1.03868600
F	7.75686300	2.65144900	-1.05150300
F	6.18442600	3.45230700	0.22903600
S	3.69373200	-0.48476400	2.98184600
H	4.43749700	1.79204100	0.91955100
H	1.90341400	-0.19694300	-0.18400700
H	0.40558700	-0.02651200	1.47143800
C	2.54479800	1.92521800	4.44945700
H	2.28505500	1.55734800	5.43867100
H	3.01764900	0.78617500	3.85087800
H	3.49744600	2.45079300	4.40324100

C	-1.76971300	0.25016200	3.84712900
H	-2.39508500	1.00020400	4.34724600
H	-2.12246300	-0.73981100	4.15841800
H	-1.91583500	0.34019600	2.76756500
C	-0.15864000	0.16649600	5.74575200
H	-0.46384300	-0.86249000	5.97027700
H	-0.81318000	0.83603800	6.31575900
H	0.86213300	0.28800000	6.12139400

TS-EF-1R-1

l imaginary frequencies

H = -5198.724349

G = -5198.915022

E(M06-2X-DCM) = -5199.559749

O	1.89283600	2.09051100	0.08248400
O	2.58706100	-0.12568700	-1.08452600
P	1.41116700	0.54266500	-0.17043000
O	1.25858300	-0.05170800	1.20012100
C	1.73938600	4.66951200	-3.20740700
C	2.78468900	3.76423900	-3.06850000
C	2.91155200	2.99744000	-1.90123200
C	0.84262700	3.96273900	-1.04255300
C	0.81213600	4.79690500	-2.17359600
C	3.93934300	-0.04807000	-0.74666400
C	4.66508300	1.09982300	-1.07385700
C	6.01151300	1.18447500	-0.67842600
C	6.64384500	0.12322000	-0.04208100
C	5.91966100	-1.03867100	0.21033600
C	4.55934100	-1.14923200	-0.12197200
H	0.01799700	5.53354200	-2.24919400
H	6.40183300	-1.88568000	0.68949600
C	4.28793500	2.34176800	-1.88199300
C	4.52016800	2.15802700	-3.41682500
H	5.57770100	2.03033200	-3.67020000
H	3.97755500	1.26608000	-3.74806100
H	7.21073300	2.94935200	-0.22587400
H	7.23679900	2.46619200	-1.91958700
C	1.88772600	3.02020100	-0.96057300
H	1.64329800	5.27727700	-4.10343500
H	7.68750600	0.19466600	0.25357400
C	3.88368700	3.41795300	-4.05081200
H	4.61356200	4.23340000	-4.15133000
H	3.48658200	3.22376500	-5.05326100
C	6.59378500	2.53328500	-1.03059400

C	5.33161400	3.36685300	-1.31233300
H	5.50313100	4.20647300	-1.99183200
H	4.94310900	3.77486200	-0.37177100
C	3.87500600	-2.44648900	0.18341400
C	3.59002500	-3.35847100	-0.86210800
C	3.65628400	-2.82088200	1.53155700
C	3.84533300	-3.06246600	-2.23881800
C	3.05636700	-4.66492700	-0.54575500
C	3.14664800	-4.13929000	1.83523500
C	3.57046700	-3.97087300	-3.22704000
H	4.26018300	-2.09531000	-2.49784900
C	2.77544700	-5.58053800	-1.60804100
C	2.85274700	-5.01971400	0.79093200
C	3.02236300	-5.24636000	-2.91209300
H	3.76783100	-3.71541600	-4.26435000
H	2.36860000	-6.55620400	-1.35212800
H	2.46906800	-6.01090800	1.02448900
H	2.80715900	-5.95159300	-3.71021000
C	-0.18699700	4.13888100	0.02885200
C	0.20630200	4.55175900	1.32930800
C	-1.56461400	3.98884000	-0.27806700
C	1.57214200	4.77418500	1.69905300
C	-0.80064000	4.79774300	2.33805600
C	-2.56063600	4.27796100	0.73112500
C	1.92063100	5.16320000	2.96636800
H	2.34483500	4.63808600	0.95201300
C	-0.39576300	5.19708800	3.65157500
C	-2.15281400	4.66307800	2.01032100
C	0.92614900	5.36910800	3.96436600
H	2.96680900	5.32423000	3.21248700
H	-1.17009700	5.37482900	4.39473800
H	-2.90640300	4.87047800	2.76767300
H	1.21971400	5.68009200	4.96356100
C	3.75987700	-2.35675000	3.92967000
H	3.99288000	-1.67695700	4.74512200
C	3.93370600	-1.94717800	2.63288800
H	4.28619900	-0.94366900	2.42604000
C	3.27426900	-3.66374700	4.22294700
H	3.14824900	-3.97317100	5.25733400
C	2.96734800	-4.52200100	3.20181700
H	2.58839100	-5.51986200	3.41009300
C	-3.36997500	3.42308200	-1.82698300
H	-3.68810800	3.05134400	-2.79606000
C	-4.34605800	3.75395400	-0.84432300

H	-5.40115700	3.65464700	-1.08311800
C	-3.94816400	4.15977800	0.40174800
H	-4.68032600	4.39916900	1.16959300
C	-2.03175100	3.53819500	-1.55543200
H	-1.31108100	3.26278300	-2.31440600
N	0.05183300	0.42499200	-1.03700800
S	-0.21137700	0.38306300	-2.62439400
C	0.17206700	-1.39431500	-3.12028300
O	0.70566500	1.18981500	-3.43818500
O	-1.65813000	0.49868200	-2.83898300
F	1.46470000	-1.53406700	-3.41798300
F	-0.13298600	-2.25070700	-2.12346600
F	-0.55646200	-1.71851200	-4.19086600
C	-0.00250700	0.32872500	4.72059300
C	-0.00288200	-1.21448000	4.44203100
H	0.42181000	-1.70598500	5.33262300
H	0.71725700	-1.41666000	3.64853100
C	-1.28116100	-2.99870900	3.10313600
C	-0.46991600	-2.88790900	1.95094600
C	-2.14943800	-4.11153200	3.20079600
C	-0.56867200	-3.82245300	0.92265900
H	0.19786800	-2.04330100	1.81587000
C	-2.22528500	-5.05303400	2.18199600
H	-2.74184600	-4.25725500	4.09823400
C	-1.44885900	-4.90139000	1.02929300
H	0.03781600	-3.69649600	0.03185900
H	-2.89375300	-5.90318100	2.28294800
H	-1.53078200	-5.61929000	0.21840700
C	-1.28138400	-1.96088700	4.14296900
C	-1.02645500	1.10035800	3.83683400
H	-2.00274300	1.14376900	4.31798400
H	-0.67734700	2.13473300	3.72742300
N	-1.22080200	0.53842100	2.50049100
C	-2.40092700	0.30432200	1.90161900
N	-2.38528300	0.10093900	0.57282300
C	-3.45056100	-0.42680700	-0.21632800
C	-3.21780300	-1.60487100	-0.92344100
C	-4.66835000	0.23918900	-0.34806600
C	-4.21016700	-2.12500000	-1.75345400
C	-5.65585600	-0.29309600	-1.17767600
H	-4.83181900	1.17538900	0.17056300
C	-5.43646400	-1.47642100	-1.88435300
H	-6.20609800	-1.88182500	-2.52882400
C	-6.93908700	0.47520100	-1.34821100

C	-3.91519700	-3.40211800	-2.49370000
F	-6.76020900	1.57698000	-2.12011300
F	-7.90444300	-0.26431000	-1.93270600
F	-7.41977000	0.91186500	-0.16285100
F	-3.63587700	-4.41465700	-1.63194500
F	-4.95169100	-3.80392700	-3.25816300
F	-2.83847900	-3.27486700	-3.29654500
S	-3.88049600	0.18983800	2.81761700
H	-2.26165600	-2.10542800	-0.83270600
H	-1.49521200	0.24235300	0.05288800
H	-0.36226600	0.42743100	1.93473900
C	-2.48022200	-1.65922700	4.80055200
H	-2.43709800	-1.09235100	5.72671100
H	-3.06586300	-0.79478400	3.96682400
H	-3.28463900	-2.39297800	4.76486800
C	1.42826500	0.83055400	4.41758100
H	2.16113500	0.29144800	5.02983400
H	1.51383900	1.89795100	4.65228200
H	1.69249500	0.68622200	3.36629500
C	-0.30915000	0.67168100	6.19442700
H	-0.26052400	1.75659100	6.34624300
H	0.43256000	0.21437200	6.85928900
H	-1.30128600	0.34400700	6.52034200

TS-EF-1R-2

l imaginary frequencies

H = -5198.722679

G = -5198.915084

E(M06-2X-DCM) = -5199.559568

O	-2.03074200	-1.93630200	0.48898900
O	-2.73226600	0.09001600	-0.97093700
P	-1.51390400	-0.47599100	-0.04733600
O	-1.23944700	0.33414600	1.18752900
C	-2.33809000	-4.93619000	-2.41287600
C	-3.33509000	-3.97568400	-2.28474200
C	-3.29835200	-3.04377800	-1.23535700
C	-1.17487600	-3.98020300	-0.48354800
C	-1.29731700	-4.95890000	-1.48466500
C	-4.04247500	0.18871000	-0.50614900
C	-4.85957800	-0.94184500	-0.54161600
C	-6.15491200	-0.86328900	-0.00518700
C	-6.65983700	0.34244100	0.46820100
C	-5.85760900	1.47961000	0.40879800
C	-4.53400000	1.43205200	-0.06266400

H	-0.53550700	-5.73003900	-1.54709800
H	-6.24772000	2.43493600	0.74693900
C	-4.63964300	-2.32120400	-1.15768600
C	-5.06061300	-2.36960600	-2.66356000
H	-6.13693200	-2.22906000	-2.80447200
H	-4.53935400	-1.56805600	-3.19785100
H	-7.35608100	-2.44403300	0.89989800
H	-7.57858300	-2.26796600	-0.83793300
C	-2.17435100	-2.98991500	-0.41481200
H	-2.36946700	-5.66872600	-3.21542300
H	-7.66744100	0.40365600	0.87171200
C	-4.54814100	-3.74105700	-3.16009500
H	-5.30291500	-4.52784800	-3.02288100
H	-4.29364600	-3.73319900	-4.22609200
C	-6.83045600	-2.21538400	-0.03434500
C	-5.64838200	-3.16649900	-0.30393100
H	-5.93971000	-4.09622800	-0.80137200
H	-5.16657800	-3.43326700	0.64399200
C	-3.74892800	2.70488300	-0.10200300
C	-3.40330400	3.28917700	-1.34609000
C	-3.46549700	3.38700400	1.10794000
C	-3.68540000	2.66791800	-2.60445900
C	-2.76593800	4.58681000	-1.37109800
C	-2.85003500	4.69414000	1.06520300
C	-3.33942000	3.26319600	-3.78833200
H	-4.17855000	1.70363800	-2.61647600
C	-2.42081400	5.17334600	-2.62902300
C	-2.51658600	5.25568500	-0.16974300
C	-2.69341900	4.53127400	-3.80574600
H	-3.55571800	2.76101200	-4.72713400
H	-1.93734400	6.14760500	-2.62641400
H	-2.05280900	6.23973700	-0.19695800
H	-2.42254100	4.98465100	-4.75527800
C	-0.02926600	-4.05353500	0.47452300
C	-0.26986400	-4.28146800	1.85478300
C	1.30142400	-3.99983100	-0.01275800
C	-1.58475200	-4.38791200	2.41281100
C	0.84807200	-4.44628200	2.75740800
C	2.40575300	-4.22841300	0.89295200
C	-1.78247600	-4.59054200	3.75396100
H	-2.44116200	-4.31135300	1.75368400
C	0.59983200	-4.64964200	4.15211300
C	2.15088000	-4.43173400	2.25129300
C	-0.67684500	-4.71284300	4.64285600

H	-2.79379200	-4.66610500	4.14455700
H	1.45556900	-4.76588200	4.81350000
H	2.98638100	-4.58886500	2.93076700
H	-0.85172500	-4.87399800	5.70335800
C	-3.51182400	3.54179800	3.54940100
H	-3.75902500	3.10327500	4.51301600
C	-3.76253600	2.83910100	2.39867300
H	-4.18923500	1.84486700	2.45814600
C	-2.92866900	4.84036200	3.49836600
H	-2.74387700	5.38648600	4.41985400
C	-2.60032900	5.39111800	2.28897700
H	-2.14411300	6.37682100	2.23375800
C	2.91060500	-3.70876000	-1.82906100
H	3.11779900	-3.46312400	-2.86635200
C	3.98945900	-3.99796900	-0.94599200
H	5.00897500	-3.99169100	-1.31903700
C	3.74112500	-4.23653800	0.37939000
H	4.55741400	-4.43513300	1.07048600
C	1.61584700	-3.70910000	-1.38047700
H	0.81390800	-3.45223900	-2.06017500
N	-0.26616000	-0.74688400	-1.03892300
S	0.14111500	0.04629500	-2.36703100
C	-0.84185900	-0.75597800	-3.75047600
O	1.53177200	-0.29952900	-2.69121100
O	-0.25628200	1.46333200	-2.39093600
F	-0.73356700	-2.09185300	-3.69199200
F	-2.14162700	-0.43448700	-3.68379900
F	-0.36052500	-0.33800700	-4.92516600
C	0.00324100	0.56370500	4.62818800
C	0.06249400	2.00679900	4.02320300
H	-0.38190800	2.68985300	4.76520300
H	-0.62225400	2.04400300	3.17527900
C	1.42022300	3.45898600	2.39558400
C	0.65046200	3.12593800	1.25841100
C	2.29667400	4.56554500	2.30589400
C	0.79779700	3.83316300	0.06674400
H	-0.02919300	2.28051600	1.27299000
C	2.41460300	5.28939400	1.12565900
H	2.85853000	4.88127000	3.17927700
C	1.68066200	4.91332800	-0.00372100
H	0.23231600	3.52162900	-0.80620300
H	3.08434500	6.14364100	1.08273000
H	1.79779800	5.45890500	-0.93544400
C	1.37093800	2.64655200	3.61984700

C	0.98000400	-0.42875200	3.92475500
H	1.94775200	-0.43908300	4.42453900
H	0.56487900	-1.44110300	4.00832200
N	1.22718100	-0.15909700	2.50591900
C	2.42807000	-0.08460300	1.91567000
N	2.47889100	-0.16004800	0.56999500
C	3.62069600	0.18312600	-0.22769000
C	3.55312000	1.30589200	-1.05198700
C	4.76987900	-0.60571200	-0.20223600
C	4.65157400	1.64722000	-1.84132000
C	5.86581500	-0.24940300	-0.98922800
H	4.79900800	-1.49745300	0.41047800
C	5.81299500	0.87672100	-1.81051200
H	6.66567000	1.14861600	-2.42144500
C	7.13805100	-1.04998600	-0.90730700
C	4.56623300	2.83267600	-2.76752300
F	6.90055300	-2.35073500	-0.61475900
F	7.82915300	-1.01523800	-2.06692200
F	7.96260200	-0.57991400	0.05657900
F	3.75884500	3.79840300	-2.27018100
F	5.78258200	3.39087200	-2.97102900
F	4.08059900	2.49398000	-3.97793900
S	3.88647800	0.16826100	2.84028700
H	2.65378500	1.90863900	-1.07461100
H	1.62188700	-0.40633700	0.05607900
H	0.38135400	-0.11474000	1.91157800
C	2.54521600	2.45291200	4.35005900
H	2.47789900	2.08549400	5.37010900
H	3.10984400	1.38413600	3.71705800
H	3.38283000	3.12501000	4.16790100
C	-1.45400200	0.07605300	4.45234500
H	-2.15061100	0.76845400	4.94014200
H	-1.58268600	-0.91013600	4.91382200
H	-1.72945100	0.00410100	3.39713200
C	0.31538600	0.52676200	6.14040500
H	0.20081500	-0.49459400	6.52302900
H	-0.38441700	1.16355900	6.69354100
H	1.33159300	0.84938800	6.38576500

TS-EF-1R-3

l imaginary frequencies

H = -5198.721004

G= -5198.912222

E(M06-2X-DCM) = -5199.556062

O	-3.10675300	-0.18737400	-1.14206800
O	-1.97429100	-1.96082700	0.38085500
P	-1.72032800	-0.51114100	-0.33516000
O	-1.44205500	0.45513000	0.78304300
C	-6.69891100	0.17840000	0.97599800
C	-6.20573600	-1.07347000	0.62410500
C	-5.04188100	-1.19151500	-0.15092600
C	-4.80613400	1.23929900	-0.16018500
C	-6.01634600	1.31770200	0.55138600
C	-2.24526700	-3.11327100	-0.35417900
C	-3.51946200	-3.31435600	-0.88434600
C	-3.72530700	-4.38298000	-1.77198000
C	-2.72101600	-5.31546900	-2.00746400
C	-1.50441900	-5.18169500	-1.33971600
C	-1.23066100	-4.07898100	-0.51263400
H	-6.41128600	2.30166100	0.78623700
H	-0.73153800	-5.93327400	-1.46937700
C	-4.85848900	-2.64040800	-0.59003900
C	-5.59270100	-3.37493400	0.58480800
H	-4.90045200	-3.46276300	1.43047500
H	-5.91367400	-4.38466000	0.31153900
H	-5.75874000	-5.12210800	-1.94649300
H	-5.11792200	-4.46189600	-3.44671900
C	-4.31517400	-0.04545600	-0.46827500
H	-7.60960900	0.27375400	1.56215500
H	-2.88379500	-6.15025800	-2.68449800
C	-6.76028100	-2.43941800	0.96376600
H	-7.04774800	-2.52644700	2.01801800
H	-7.66016100	-2.66270400	0.37356900
C	-5.11949200	-4.32887600	-2.35877500
C	-5.61038600	-2.92812700	-1.93229400
H	-5.30056600	-2.18353600	-2.67429600
H	-6.69755900	-2.86192400	-1.82512400
C	0.07940000	-4.01498100	0.20728500
C	1.29255300	-3.98663500	-0.52543900
C	0.11038600	-4.09961600	1.62438200
C	1.33422400	-3.87815400	-1.95286100
C	2.55628100	-4.06055100	0.17492400
C	1.38205700	-4.13484000	2.31191200
C	2.52284100	-3.89029200	-2.63456100
H	0.40546600	-3.75026800	-2.49463200
C	3.77443300	-4.06789900	-0.57531500
C	2.56726100	-4.11968500	1.57090500
C	3.76176300	-3.99343500	-1.94187700

H	2. 52112800	-3. 78808600	-3. 71599400
H	4. 71486300	-4. 12108900	-0. 03281600
H	3. 52049000	-4. 17242700	2. 09343000
H	4. 69569900	-3. 98463200	-2. 49573700
C	-4. 12652300	2. 50137200	-0. 58717500
C	-3. 68955600	3. 43125700	0. 38988500
C	-4. 01054700	2. 81285900	-1. 96570000
C	-3. 77073200	3. 18060100	1. 79864200
C	-3. 13642300	4. 70045500	-0. 02676800
C	-3. 41697100	4. 06831000	-2. 36648500
C	-3. 39146400	4. 12544800	2. 71794500
H	-4. 14232900	2. 22089500	2. 13724100
C	-2. 74632000	5. 65506200	0. 96459200
C	-3. 00188900	4. 97677500	-1. 38970500
C	-2. 87906300	5. 38650600	2. 29978300
H	-3. 48169000	3. 91029800	3. 77994900
H	-2. 34268900	6. 60729000	0. 62822100
H	-2. 57843900	5. 93060800	-1. 69874900
H	-2. 58755300	6. 12515300	3. 04173200
C	-1. 00689200	-4. 28114900	3. 79593100
H	-1. 92355000	-4. 36072600	4. 37467300
C	-1. 07177800	-4. 19308500	2. 42870900
H	-2. 03837000	-4. 20937500	1. 93955600
C	0. 24936200	-4. 28582300	4. 46700900
H	0. 28303300	-4. 35898800	5. 55089700
C	1. 40731000	-4. 21759900	3. 74002400
H	2. 37554700	-4. 23610800	4. 23475700
C	-4. 36415200	2. 28511600	-4. 32495900
H	-4. 73380100	1. 60737100	-5. 08958300
C	-3. 74865900	3. 50803600	-4. 71308100
H	-3. 64736500	3. 74941400	-5. 76759200
C	-3. 29405900	4. 37418400	-3. 75756800
H	-2. 83162000	5. 31790200	-4. 03703300
C	-4. 49165300	1. 95182800	-3. 00291500
H	-4. 96976100	1. 01829800	-2. 73165200
N	-0. 62234700	-0. 73384000	-1. 49542300
S	-0. 02501800	0. 50780300	-2. 29364800
O	0. 79107100	1. 40895400	-1. 42154500
O	-0. 91657300	1. 17186000	-3. 24749100
C	1. 25566700	-0. 36775200	-3. 32690400
F	2. 25640800	-0. 81187200	-2. 55500000
F	1. 75404900	0. 50754300	-4. 20695500
F	0. 72729400	-1. 39665200	-3. 99648900
C	-0. 58215500	0. 60714600	4. 42218700

C	-0.37788400	2.11550200	4.05654400
H	-0.81375000	2.70787600	4.87728700
H	-1.00080400	2.34307700	3.19049900
C	1.19442100	3.61948800	2.69760700
C	0.50556900	3.45203300	1.47581600
C	2.11480600	4.68745200	2.80248700
C	0.76279300	4.28984000	0.39358200
H	-0.19707700	2.63767700	1.33588800
C	2.34401600	5.54147800	1.73012500
H	2.62070600	4.87278500	3.74469200
C	1.67805900	5.33743400	0.51775400
H	0.25293000	4.10550700	-0.54601800
H	3.04293200	6.36603800	1.83811100
H	1.87089900	5.99475700	-0.32565800
C	0.99897700	2.69420900	3.82542100
C	0.39794200	-0.34194100	3.66422500
H	1.28225500	-0.54229300	4.26725400
H	-0.10553100	-1.30197100	3.50222800
N	0.86010200	0.13671000	2.35843200
C	2.13610100	0.19407500	1.95556100
N	2.37542200	0.40331900	0.64747500
C	3.65444800	0.50338400	0.03180400
C	3.93690900	1.62271800	-0.75331400
C	4.58573100	-0.53173000	0.14204700
C	5.16952900	1.71389800	-1.40198800
C	5.81446100	-0.42472900	-0.50645600
H	4.34097200	-1.41988900	0.71003500
C	6.11661300	0.69862500	-1.27777500
H	7.07258700	0.77665200	-1.78238700
C	6.79927000	-1.56253700	-0.44645300
C	5.50667000	2.95809800	-2.18237100
F	6.69607000	-2.37264500	-1.52796800
F	8.07387500	-1.11775900	-0.41538900
F	6.61198200	-2.34024000	0.64402700
F	6.06989900	3.90002000	-1.38798700
F	6.38786600	2.70399600	-3.17396000
F	4.41199400	3.51583800	-2.73753900
S	3.45340600	0.12029200	3.10685600
H	3.19440000	2.40408100	-0.86379300
H	1.59133100	0.63388900	0.01241900
H	0.10842300	0.22821300	1.64747400
C	2.08122500	2.36769400	4.64284700
H	1.88919900	1.92295100	5.61580100
H	2.66321700	1.30350100	3.98970400

H	2.96957600	2.99643700	4.60056400
C	-2.04125600	0.26177200	4.04602500
H	-2.74082300	0.93424900	4.55791700
H	-2.27951000	-0.76337400	4.35323100
H	-2.20494600	0.34232600	2.96788400
C	-0.41585100	0.33013400	5.93218600
H	-0.60546100	-0.72919300	6.14281700
H	-1.13608500	0.91545900	6.51544000
H	0.58736800	0.55733900	6.30576500

TS-EF-1R-4

1 imaginary frequencies

H = -5198.723060

G = -5198.916123

E(M06-2X-DCM) = 5199.558647

O	-3.12427100	0.20378000	-0.97075300
O	-2.35951700	-1.54092800	0.78266200
P	-1.80877100	-0.30372500	-0.14065400
O	-1.25083000	0.70971900	0.81785000
C	-6.47952700	1.59802900	1.10994400
C	-6.27221800	0.23436600	0.93140400
C	-5.19064400	-0.23151900	0.16795700
C	-4.45186600	2.07128900	-0.17886400
C	-5.59135200	2.49956800	0.52503600
C	-2.86782600	-2.69617600	0.19131900
C	-4.17740300	-2.70311800	-0.28599000
C	-4.62519600	-3.80392200	-1.03366800
C	-3.82478500	-4.93044600	-1.18830500
C	-2.56760100	-4.95521000	-0.58509400
C	-2.05354900	-3.84288600	0.10223700
H	-5.76246000	3.56722800	0.62533500
H	-1.94896100	-5.84445000	-0.66161900
C	-5.33500800	-1.73272100	-0.06528800
C	-6.15560100	-2.12909300	1.20964900
H	-5.46210300	-2.24761800	2.05041600
H	-6.69198700	-3.07465300	1.08451700
H	-6.77107500	-4.12901400	-1.05689900
H	-6.09018200	-3.81201000	-2.64866200
C	-4.25300600	0.68243100	-0.31157600
H	-7.32675500	1.96169000	1.68613000
H	-4.17349700	-5.78725700	-1.75930400
C	-7.08503700	-0.92395200	1.46700800
H	-7.33947900	-0.80396800	2.52647400
H	-8.03584700	-1.02845400	0.92571400

C	-6.00864000	-3.54313200	-1.58927800
C	-6.18807800	-2.02890900	-1.34453600
H	-5.76767700	-1.46504800	-2.18505400
H	-7.23380700	-1.72730100	-1.22925400
C	-0.70449000	-3.94350600	0.74257300
C	0.44610600	-4.15841800	-0.05633700
C	-0.59205100	-3.93010200	2.15685000
C	0.40840900	-4.13810900	-1.48787700
C	1.72642500	-4.38845200	0.57606400
C	0.70093000	-4.12797800	2.77397800
C	1.53418000	-4.36545600	-2.23460400
H	-0.52374900	-3.89686900	-1.98146300
C	2.87568600	-4.63417900	-0.24079000
C	1.82086500	-4.35856500	1.96968700
C	2.78452400	-4.63215900	-1.60757300
H	1.47902900	-4.31527800	-3.31781200
H	3.83030300	-4.81123600	0.24927000
H	2.78741800	-4.52543400	2.44092100
H	3.66910000	-4.79935400	-2.21480100
C	-3.53494800	3.09014600	-0.77644400
C	-2.88625100	4.03045400	0.06351900
C	-3.38556500	3.17445900	-2.18389900
C	-2.97244100	3.99092400	1.49378300
C	-2.09202900	5.08611700	-0.52358400
C	-2.55362700	4.21003900	-2.75288400
C	-2.37152800	4.94509500	2.27463500
H	-3.52394600	3.18413600	1.96162100
C	-1.47925800	6.05914400	0.32707500
C	-1.93899500	5.14005400	-1.91106600
C	-1.62064200	6.00257000	1.68687200
H	-2.46687400	4.89383900	3.35654200
H	-0.89467400	6.85002000	-0.13709800
H	-1.33310800	5.93160900	-2.34786900
H	-1.15542100	6.75291200	2.32060500
C	-1.57465500	-3.75129500	4.39207900
H	-2.44963300	-3.62555300	5.02460000
C	-1.71668300	-3.75775900	3.02792300
H	-2.70238100	-3.64166700	2.59282600
C	-0.29412800	-3.92272600	4.99191300
H	-0.19994500	-3.91858900	6.07466000
C	0.80752100	-4.10898300	4.20074900
H	1.79021600	-4.25540600	4.64301400
C	-3.87785200	2.39694400	-4.44858800
H	-4.39292300	1.70810800	-5.11270500

C	-3.03209700	3.40014800	-5.00015800
H	-2.90193300	3.46345000	-6.07705700
C	-2.39562300	4.28315700	-4.17203900
H	-1.75565500	5.06318200	-4.57776000
C	-4.05153500	2.29238800	-3.09379100
H	-4.71008200	1.52840500	-2.69845900
N	-0.84331600	-0.96409800	-1.24571200
S	0.08479000	-0.12129200	-2.21906500
O	1.50293700	-0.51472100	-2.03573300
O	-0.20037000	1.32088400	-2.31289100
C	-0.37434100	-0.80891500	-3.89242100
F	-0.19166200	-2.13602200	-3.94190300
F	0.39308600	-0.23733000	-4.82672800
F	-1.65600500	-0.54201200	-4.15722200
C	-0.16969100	0.99817400	4.27364500
C	0.19367700	2.39302200	3.65886700
H	-0.13791300	3.15379900	4.38331000
H	-0.43599900	2.54737400	2.78251600
C	1.90037900	3.40778300	2.01875900
C	1.12464200	3.13932800	0.86819400
C	3.00438800	4.28325900	1.88454400
C	1.47390200	3.67354600	-0.36984600
H	0.27238600	2.47008300	0.90868900
C	3.33263800	4.83819100	0.65301900
H	3.58557300	4.55972700	2.75835400
C	2.57719300	4.52210300	-0.48097300
H	0.88762800	3.39994000	-1.24130200
H	4.18150700	5.51102200	0.57491900
H	2.84896800	4.93844300	-1.44705900
C	1.61897800	2.75648700	3.30829800
C	0.59594300	-0.19519300	3.60717200
H	1.44372500	-0.49425300	4.22212200
H	-0.08268300	-1.05311300	3.55022300
N	1.11128500	0.03968400	2.25430800
C	2.38121500	-0.12874300	1.86309000
N	2.64447200	-0.23264300	0.54740100
C	3.94043500	-0.17290100	-0.05305900
C	4.72158700	0.98140200	0.03237300
C	4.37783100	-1.26524200	-0.79774600
C	5.96204800	1.01863900	-0.60196100
C	5.62092200	-1.21336400	-1.43266000
H	3.74931900	-2.14472700	-0.88202200
C	6.42178300	-0.07832400	-1.33471900
H	7.38381200	-0.04159900	-1.83017000

C	6.07286000	-2.41636900	-2.21900700
C	6.82419100	2.24462000	-0.45621400
F	5.24548600	-2.67675100	-3.25466500
F	7.31558700	-2.26286900	-2.72078200
F	6.08435400	-3.53146000	-1.44673900
F	7.51081900	2.23580400	0.71000500
F	7.73244600	2.34598500	-1.44933400
F	6.08567400	3.37899400	-0.46272100
S	3.69142200	-0.17468300	3.01994900
H	4.35709600	1.84364900	0.57785900
H	1.89400200	-0.40101200	-0.13554900
H	0.37472000	0.19068700	1.54361700
C	2.67217100	2.45505700	4.17130200
H	2.45105000	2.22921500	5.21048400
H	3.08544700	1.21355300	3.71615900
H	3.63509700	2.93703000	4.01074000
C	-1.69203700	0.82361700	4.06467600
H	-2.24170700	1.65098000	4.53064900
H	-2.03466800	-0.10802200	4.53001300
H	-1.94438800	0.79052000	3.00200000
C	0.09197500	0.91874500	5.79415700
H	-0.26031500	-0.04442400	6.18243100
H	-0.45509400	1.70648200	6.32509700
H	1.15034900	1.00031300	6.05841200

TS-EF-1R-5

l imaginary frequencies

H = -5198.730764

G = -5198.922840

E(M06-2X-DCM) = -5199.559918

O	-3.08809100	0.01473100	-0.29653300
O	-1.61264900	-2.09961200	-0.11395900
P	-1.51985700	-0.47774000	-0.27777000
O	-0.77335200	0.05207800	0.90431600
C	-5.49921700	-0.95532000	2.99349300
C	-5.33587200	-1.84943000	1.94128000
C	-4.57313000	-1.50325000	0.81515400
C	-4.05589200	0.64985600	1.84151900
C	-4.87681500	0.28957700	2.92381600
C	-2.18102100	-2.87239200	-1.12665800
C	-3.56833100	-2.95876000	-1.22847200
C	-4.13383100	-3.56831900	-2.35921100
C	-3.32860100	-4.20954400	-3.29441100
C	-1.94844100	-4.23954100	-3.09258600

C	-1.33920700	-3.56005100	-2.02385500
H	-5.00109000	1.00232700	3.73392300
H	-1.31313000	-4.77750500	-3.78980900
C	-4.67665300	-2.59833500	-0.24217500
C	-5.00167900	-3.83110500	0.67243500
H	-4.06258000	-4.21940900	1.08329600
H	-5.48507400	-4.64362100	0.12166300
H	-6.14881300	-4.34790900	-2.13227700
H	-6.02132300	-3.06138200	-3.32608700
C	-3.90438400	-0.27920100	0.79357600
H	-6.09596400	-1.22081600	3.86250600
H	-3.76344200	-4.69529100	-4.16445400
C	-5.86703400	-3.25920600	1.81317800
H	-5.77488800	-3.83040700	2.74395800
H	-6.93347600	-3.26007400	1.54630800
C	-5.63900200	-3.40044200	-2.35635200
C	-5.86177400	-2.36045200	-1.23416300
H	-5.78056000	-1.34721400	-1.64389700
H	-6.83881200	-2.44863600	-0.74824900
C	0.14547400	-3.62824200	-1.85389300
C	1.00212100	-3.14709100	-2.87641300
C	0.69560900	-4.26079400	-0.70889000
C	0.51868300	-2.47323800	-4.04457900
C	2.43219200	-3.32263800	-2.75266600
C	2.13040500	-4.37589600	-0.57481000
C	1.36811100	-2.07390700	-5.04285000
H	-0.53902200	-2.25469500	-4.12111500
C	3.28451900	-2.89703100	-3.81987500
C	2.95815900	-3.90887400	-1.59892800
C	2.76972700	-2.30572800	-4.94287700
H	0.97137400	-1.55641600	-5.91149700
H	4.35435900	-3.06757900	-3.71951800
H	4.03697500	-4.00380600	-1.49448500
H	3.42552900	-2.00041400	-5.75463800
C	-3.40346300	1.99721200	1.86765100
C	-2.40760400	2.27006500	2.83704300
C	-3.85872600	3.02516400	1.00700400
C	-1.87846300	1.26258300	3.70814300
C	-1.88172900	3.61014500	2.96613700
C	-3.31452400	4.35816100	1.13581700
C	-0.92626300	1.55821100	4.64925000
H	-2.23151900	0.24441300	3.59986700
C	-0.89356200	3.87849900	3.96641100
C	-2.35194500	4.61635000	2.11665300

C	-0.42876700	2.88650400	4.78705100
H	-0.53760800	0.77010300	5.28914200
H	-0.51927800	4.89567400	4.06047000
H	-1.97078200	5.62995700	2.23164600
H	0.32306700	3.10441100	5.54065400
C	0.45586600	-5.41524000	1.43481500
H	-0.18158300	-5.82858900	2.21152100
C	-0.10751000	-4.82669400	0.33347600
H	-1.18652700	-4.79052000	0.24220300
C	1.87010100	-5.49067600	1.57712400
H	2.29749500	-5.95306400	2.46278100
C	2.68028600	-4.99037000	0.59448400
H	3.76229400	-5.04090400	0.68621000
C	-5.29998500	3.83211900	-0.79378400
H	-6.06632000	3.64178900	-1.54020500
C	-4.75273800	5.14055300	-0.66991300
H	-5.10572800	5.93559300	-1.32124500
C	-3.79174300	5.39266200	0.27142700
H	-3.37490300	6.39115400	0.38467000
C	-4.87219200	2.81479600	0.01817900
H	-5.30385800	1.82599500	-0.08509400
N	-0.99832200	-0.22795700	-1.78887700
S	-0.59020400	1.14402900	-2.43562800
O	0.44823800	0.97986900	-3.46184100
O	-0.38817300	2.26358700	-1.46938900
C	-2.09000300	1.69709200	-3.40383000
F	-2.39414400	0.78916900	-4.33757500
F	-1.81831500	2.86317000	-4.00808300
F	-3.14213200	1.86390500	-2.59912500
C	1.54959800	5.48212600	-0.62499000
C	2.54636300	4.85256400	-1.65253300
H	2.87032300	5.66160700	-2.32881000
H	1.98590500	4.17043900	-2.29342600
C	4.26837800	2.99463400	-1.97924600
C	3.34319800	2.08587500	-2.54016600
C	5.64890600	2.72483500	-2.13780600
C	3.77793400	0.94102500	-3.20031900
H	2.27538100	2.22435900	-2.42584000
C	6.07876300	1.59488600	-2.82180700
H	6.38434000	3.43002100	-1.76398800
C	5.14441500	0.69417400	-3.34502100
H	3.03960100	0.24888100	-3.59082800
H	7.14241900	1.41543900	-2.94983900
H	5.48016300	-0.19797800	-3.86601000

C	3. 81953900	4. 16609800	-1. 22329400
C	1. 40530500	4. 64454300	0. 67824300
H	2. 18211400	4. 90585900	1. 39625400
H	0. 44285400	4. 89868500	1. 14070500
N	1. 44877700	3. 19362700	0. 50000700
C	2. 14976700	2. 32883400	1. 25750600
N	1. 72265000	1. 05567500	1. 26534500
C	2. 39671300	-0. 05116600	1. 85813400
C	3. 59926200	-0. 52931500	1. 33744000
C	1. 77419700	-0. 71202500	2. 91889100
C	4. 19295300	-1. 65659300	1. 90677700
C	2. 38070000	-1. 83370400	3. 48193400
H	0. 82490600	-0. 34340500	3. 28894700
C	3. 59448700	-2. 30815600	2. 98490200
H	4. 06007800	-3. 18265800	3. 42214000
C	1. 69351100	-2. 57305000	4. 59986600
C	5. 50067500	-2. 15618200	1. 35341500
F	0. 91472300	-1. 75125000	5. 34125600
F	0. 89572300	-3. 56034300	4. 13761500
F	2. 58575300	-3. 14885200	5. 43716800
F	6. 55417700	-1. 46193200	1. 83975100
F	5. 71462000	-3. 45828200	1. 65511200
F	5. 54801200	-2. 04314500	0. 00568900
S	3. 55267100	2. 81057000	2. 16621800
H	4. 05145100	-0. 03883000	0. 48323500
H	0. 74066300	0. 84097600	0. 98914000
H	0. 71179300	2. 78468100	-0. 08963800
C	4. 55903500	4. 59035700	-0. 11007500
H	4. 39655500	5. 59653800	0. 26825000
H	4. 07776500	3. 85049900	0. 86816700
H	5. 58951200	4. 24587600	-0. 02535700
C	0. 18604700	5. 57561200	-1. 34918300
H	0. 28227600	6. 15999800	-2. 27240700
H	-0. 55184100	6. 07864000	-0. 71377200
H	-0. 20950700	4. 59043000	-1. 61238000
C	1. 95203900	6. 91424300	-0. 21043500
H	1. 21229600	7. 32999100	0. 48416200
H	1. 98547700	7. 57337900	-1. 08530000
H	2. 92611800	6. 96498500	0. 28617400

INT-5

0 imaginary frequencies

H = -5198. 727929

G = -5198. 920989

E(M06-2X-DCM) = -5199.571873

O	1.79612400	-2.18878600	-0.14599200
O	3.10133000	-0.00075200	0.35457400
P	1.59550900	-0.56597000	0.01701100
O	0.73979200	-0.21007500	1.19336700
C	3.18561700	-4.35713100	3.16340200
C	4.07176700	-3.69161400	2.32354000
C	3.60935300	-3.03304500	1.17419700
C	1.31858600	-3.64521000	1.74601200
C	1.82799500	-4.35655900	2.84673400
C	4.14037700	-0.17410600	-0.55775800
C	4.80013200	-1.40175900	-0.62610600
C	5.72598600	-1.62654400	-1.65757500
C	6.08266000	-0.60381000	-2.52882800
C	5.51175300	0.65574100	-2.35819600
C	4.52591500	0.89918400	-1.38608100
H	1.12780000	-4.90191500	3.47261800
H	5.81350200	1.47657200	-3.00180700
C	4.79346500	-2.60118000	0.31767400
C	5.89136300	-2.44280300	1.42449900
H	5.77711800	-1.45848400	1.89362900
H	6.90617000	-2.50279100	1.01926100
H	7.24047200	-3.13030600	-1.26907300
H	6.20376800	-3.51367300	-2.63897600
C	2.23823000	-2.94987600	0.93476900
H	3.54111200	-4.88145400	4.04700200
H	6.80528400	-0.77399600	-3.32287500
C	5.57264300	-3.54938500	2.45235800
H	5.88420800	-3.28489800	3.46954000
H	6.08527600	-4.48867700	2.20148600
C	6.20855400	-3.06051200	-1.64104700
C	5.21314300	-3.73694000	-0.67475200
H	4.32511600	-4.06519200	-1.22674000
H	5.62880000	-4.60898300	-0.16040600
C	4.00087000	2.29402200	-1.25456700
C	3.34726600	2.90476600	-2.35490600
C	4.28993600	3.05567900	-0.09226300
C	2.95538000	2.17338900	-3.52335300
C	3.04011400	4.31761500	-2.31383300
C	3.92230700	4.45448000	-0.04311300
C	2.36231700	2.79954600	-4.58861600
H	3.09459700	1.09978400	-3.53910800
C	2.43821900	4.93558900	-3.45527600
C	3.32662000	5.05033100	-1.15868000

C	2. 11807900	4. 20253200	-4. 56634200
H	2. 05394900	2. 21565300	-5. 45067700
H	2. 23478900	6. 00325800	-3. 41507200
H	3. 08726500	6. 11171500	-1. 12969600
H	1. 65894700	4. 68236100	-5. 42662200
C	-0. 15091200	-3. 69073900	1. 47302600
C	-1. 06024900	-3. 15435800	2. 41823200
C	-0. 63501600	-4. 36030100	0. 32154400
C	-0. 63964700	-2. 48767600	3. 61527500
C	-2. 48253400	-3. 28180700	2. 19315000
C	-2. 05908900	-4. 44282800	0. 08923200
C	-1. 54854800	-2. 03212100	4. 53576800
H	0. 42072400	-2. 34824000	3. 78932200
C	-3. 39629000	-2. 77142100	3. 16827200
C	-2. 94262900	-3. 90495200	1. 02970600
C	-2. 94844200	-2. 17304500	4. 31438800
H	-1. 19970200	-1. 55322900	5. 44754800
H	-4. 46161500	-2. 87469400	2. 97717600
H	-4. 01296000	-3. 97500600	0. 85154000
H	-3. 65267500	-1. 79299800	5. 04857300
C	5. 23654000	3. 27791900	2. 15413800
H	5. 76235600	2. 83884500	2. 99784500
C	4. 97381300	2. 51575300	1. 04506900
H	5. 29539100	1. 48162500	1. 01940600
C	4. 84073300	4. 64527500	2. 20895300
H	5. 06118700	5. 23585500	3. 09436800
C	4. 20719600	5. 21329300	1. 13656500
H	3. 92101000	6. 26272400	1. 15279100
C	-0. 27736900	-5. 64579100	-1. 72499000
H	0. 40077900	-6. 12644300	-2. 42510900
C	-1. 67891900	-5. 68343100	-1. 97096600
H	-2. 05658600	-6. 18053700	-2. 86028600
C	-2. 54320100	-5. 09865200	-1. 08616200
H	-3. 61543700	-5. 11408300	-1. 25956500
C	0. 22533000	-5. 00512300	-0. 62321800
H	1. 29599200	-4. 98707700	-0. 45522000
C	0. 57717400	2. 42671400	3. 91045200
C	0. 60659100	3. 43556300	2. 68801700
H	1. 16058900	4. 32767800	3. 02098600
H	1. 20007700	2. 97720000	1. 89928300
C	-1. 01369100	3. 91928800	0. 74500400
C	-0. 06522000	3. 55267100	-0. 25072900
C	-2. 33577200	4. 24075400	0. 31740400
C	-0. 42522100	3. 49553800	-1. 58635000

H	0.95622300	3.31413200	0.01645200
C	-2.69617900	4.15204500	-1.01668600
H	-3.09143200	4.51000000	1.04493600
C	-1.74277300	3.77278800	-1.96941900
H	0.29687700	3.18588400	-2.32900900
H	-3.72315300	4.34497700	-1.31116200
H	-2.02412300	3.67457600	-3.01327300
C	-0.70100500	3.91665800	2.14358700
C	-0.70881100	1.55079000	3.88566300
H	-1.52168500	2.02131400	4.43942200
H	-0.49170500	0.59485300	4.37834100
N	-1.19362600	1.29045300	2.53525400
C	-2.50876000	1.15163900	2.19065900
N	-2.69296700	0.56408300	0.97337900
C	-3.90662000	0.40282600	0.25777700
C	-4.85218200	1.42690300	0.14713800
C	-4.11138300	-0.79715900	-0.43113600
C	-5.99325700	1.24082600	-0.63120800
C	-5.26513800	-0.97349800	-1.19635500
H	-3.36189300	-1.57771800	-0.38522000
C	-6.21752700	0.03882700	-1.30212600
H	-7.10317800	-0.09809200	-1.90921400
C	-5.47583900	-2.29525300	-1.88723000
C	-6.98433400	2.36839000	-0.72693900
F	-4.38240000	-2.68848100	-2.56887000
F	-6.50991000	-2.25978700	-2.75400700
F	-5.74860000	-3.28533800	-0.99229100
F	-7.74769100	2.47183400	0.38252500
F	-7.82077000	2.22623100	-1.77574300
F	-6.35691500	3.56733800	-0.87296300
S	-3.77538700	1.72440000	3.17561500
H	-4.69089000	2.36759600	0.65192500
H	-1.88994200	0.11978300	0.51851700
H	-0.51095200	0.79761800	1.93593200
C	-1.66565400	4.50455000	3.10293900
H	-1.19906100	4.75997200	4.05257600
H	-2.46484900	3.75037400	3.30936900
H	-2.17152800	5.38597900	2.70343400
N	1.26556300	-0.01290100	-1.46275500
S	-0.12399500	-0.22262200	-2.20589600
O	-0.43046400	0.91089000	-3.08885000
O	-1.20966500	-0.72850900	-1.33103500
C	0.21901200	-1.60887300	-3.41205500
F	1.19678600	-1.23841700	-4.25309800

F	-0.88389000	-1.86586700	-4.12372800
F	0.59787500	-2.72050900	-2.77851800
C	1.84168600	1.54947800	3.77426900
H	2.74130700	2.17355500	3.72099500
H	1.93833800	0.89561000	4.64940300
H	1.80713500	0.92129400	2.88039800
C	0.65213000	3.13611100	5.27879400
H	0.66828400	2.38970100	6.08165400
H	1.57294100	3.72459800	5.36195900
H	-0.19644100	3.79806800	5.47527700

INT-6

0 imaginary frequencies

H = -5198.745139

G = -5198.932271

E(M06-2X-DCM) = -5199.602155

O	-1.38398100	2.35093500	-0.20506800
O	-2.96810100	0.34501400	0.28306000
P	-1.42826000	0.71196000	-0.15756000
O	-0.53758100	0.13529000	0.90747700
C	-2.47401100	4.66285100	3.12317100
C	-3.44238900	4.11096200	2.29239400
C	-3.07798100	3.39958600	1.13817800
C	-0.72442500	3.74010600	1.67959300
C	-1.13107200	4.50497400	2.78709000
C	-4.03292200	0.64079100	-0.57386900
C	-4.50441100	1.95043200	-0.64927100
C	-5.41826000	2.29581900	-1.65696500
C	-5.95719600	1.32070300	-2.48822100
C	-5.59501700	-0.00991700	-2.28619000
C	-4.62662100	-0.38389900	-1.33788500
H	-0.36333800	4.97280600	3.39616400
H	-6.05433700	-0.79085800	-2.88456900
C	-4.31514200	3.13768800	0.28754600
C	-5.41919400	3.12707900	1.40036000
H	-5.44000100	2.13353900	1.86348800
H	-6.41738800	3.32808000	0.99998700
H	-6.68551600	4.01547900	-1.27437800
H	-5.61581100	4.22325000	-2.65624200
C	-1.72922600	3.14625800	0.88732000
H	-2.75462900	5.22803400	4.00846000
H	-6.66932000	1.58166800	-3.26694600
C	-4.94727800	4.17195900	2.43188700
H	-5.28479800	3.94562300	3.44999700

H	-5.32785800	5.17439500	2.19075000
C	-5.67943400	3.78669100	-1.65292400
C	-4.58374700	4.31916000	-0.70335200
H	-3.66628700	4.51813200	-1.26881200
H	-4.86583800	5.24213100	-0.18713400
C	-4.36546100	-1.84400700	-1.13745500
C	-3.86994900	-2.63102800	-2.20741100
C	-4.77573000	-2.46825200	0.06965100
C	-3.40313700	-2.05945800	-3.43486600
C	-3.81799500	-4.07056900	-2.07547000
C	-4.66484500	-3.90445000	0.20566500
C	-2.97216800	-2.84963800	-4.46878500
H	-3.35487700	-0.98174500	-3.52579600
C	-3.37337700	-4.85853300	-3.18289700
C	-4.20094200	-4.66482700	-0.87089400
C	-2.97379700	-4.26865300	-4.35197500
H	-2.59843700	-2.38570100	-5.37632700
H	-3.35620400	-5.94004700	-3.07027100
H	-4.14838100	-5.74733700	-0.77253400
H	-2.63743700	-4.87751200	-5.18705300
C	0.73392500	3.65067300	1.36488400
C	1.62279800	3.04897600	2.28940600
C	1.23793100	4.26636100	0.19175600
C	1.18638800	2.44799600	3.51566900
C	3.04172600	3.03992400	2.01358000
C	2.65437600	4.21380400	-0.08985100
C	2.08085800	1.92480200	4.41408000
H	0.12498900	2.42375700	3.73532000
C	3.93841300	2.46828900	2.96997400
C	3.51568800	3.59886200	0.82353700
C	3.47878300	1.93585000	4.14367000
H	1.72172200	1.49184700	5.34438700
H	5.00174100	2.47332100	2.74302700
H	4.57975700	3.56026100	0.60545100
H	4.17140700	1.51219900	4.86499500
C	-5.74827800	-2.38465300	2.31497500
H	-6.19204800	-1.80967100	3.12367300
C	-5.35189200	-1.74870700	1.16651000
H	-5.48864600	-0.67760100	1.07552700
C	-5.59680800	-3.79360400	2.45747000
H	-5.91436500	-4.28103000	3.37548800
C	-5.07282200	-4.52722000	1.42758200
H	-4.97140400	-5.60700700	1.51074800
C	0.92685500	5.55328100	-1.86194600

H	0.27152900	6.08664700	-2.54536900
C	2.31714300	5.46134700	-2.15412300
H	2.70779000	5.91323700	-3.06176700
C	3.15457600	4.81105200	-1.28962600
H	4.21725800	4.72868100	-1.49835300
C	0.40705200	4.97577900	-0.73362300
H	-0.65363000	5.06166600	-0.52843800
C	-1.10489400	-2.01115600	3.79986700
C	-1.13925100	-3.13853100	2.71761900
H	-1.52807600	-4.08096900	3.11465300
H	-1.80136600	-2.84564900	1.89962600
C	0.38967600	-3.86780100	0.75131600
C	-0.36213500	-3.26945500	-0.27180400
C	1.21853700	-4.95064400	0.41345500
C	-0.27555100	-3.72101700	-1.58751700
H	-1.01280800	-2.42730900	-0.06014700
C	1.29142400	-5.41608100	-0.89951200
H	1.81142500	-5.45281800	1.16800500
C	0.54899800	-4.79974700	-1.90477300
H	-0.83988800	-3.21855800	-2.36448700
H	1.93775000	-6.25834800	-1.13134500
H	0.61281200	-5.15075200	-2.93063700
C	0.29875500	-3.35421000	2.18686400
C	0.26682000	-1.31352800	3.57591600
H	1.00556100	-1.55760900	4.33795700
H	0.20179500	-0.22995100	3.47708300
N	0.79503000	-1.83854600	2.25746100
C	2.25560200	-1.59681100	2.00249300
N	2.46548700	-1.25999700	0.72096600
C	3.74163600	-1.03630200	0.12205500
C	4.78143700	-1.95700000	0.26592300
C	3.90504200	0.09588300	-0.68008100
C	5.99437600	-1.72931000	-0.38151300
C	5.12423200	0.30550500	-1.32596100
H	3.08459800	0.78871000	-0.81463900
C	6.17482300	-0.59922700	-1.17883300
H	7.11348700	-0.43814600	-1.69564700
C	5.32746600	1.54379700	-2.16094700
C	7.13362300	-2.69563900	-0.18534400
F	4.17669900	1.99717300	-2.68798800
F	6.19186400	1.32503500	-3.17455800
F	5.85238000	2.55919900	-1.42029900
F	7.90457000	-2.34653600	0.86921800
F	7.94164600	-2.74092800	-1.26638300

F	6.69151400	-3.95101500	0.04791900
S	3.37262000	-1.75431100	3.21143600
H	4.64337400	-2.84997800	0.85999100
H	1.67852000	-1.05505700	0.08645900
H	0.25492000	-1.29023100	1.54352900
C	1.10732300	-4.20800600	3.16970700
H	1.08657900	-3.80405700	4.18043900
H	2.15341900	-4.31154600	2.88415900
H	0.65240600	-5.20288300	3.19563900
N	-1.29612000	0.27641300	-1.69915900
S	0.01350900	-0.11343900	-2.49721300
O	-0.32666700	-0.83030100	-3.72687800
O	1.10429300	-0.67446400	-1.65829700
C	0.74299700	1.50726100	-3.07721400
F	-0.18012100	2.26636100	-3.66990700
F	1.73528500	1.27048100	-3.94088300
F	1.24151200	2.17183600	-2.02136300
C	-2.26820200	-1.02504900	3.58594700
H	-3.22784400	-1.54823600	3.65530800
H	-2.25348600	-0.24238200	4.35477400
H	-2.21459700	-0.54374100	2.60772000
C	-1.20132300	-2.56189500	5.23690700
H	-1.10034700	-1.75004800	5.96725600
H	-2.18009000	-3.02789100	5.39680800
H	-0.43494500	-3.30959300	5.46332300

TS-PT-1S

l imaginary frequencies

H = -5198.731392

G = -5198.917520

E(M06-2X-DCM) = -5199.584425

O	-1.25612300	2.36449900	-0.24258000
O	-2.88833000	0.40740800	0.32971900
P	-1.38887300	0.75528800	-0.18979300
O	-0.45013600	0.28633300	0.95341000
C	-2.16550600	4.79665600	3.06033100
C	-3.17803000	4.23763700	2.28952700
C	-2.87350700	3.48961800	1.14105600
C	-0.48962300	3.80163200	1.57388600
C	-0.84137400	4.60759100	2.67214800
C	-3.98719100	0.72693500	-0.50018100
C	-4.40684700	2.05449400	-0.57329700
C	-5.34337500	2.42246100	-1.55275700
C	-5.94427900	1.46028700	-2.35513400

C	-5.62500700	0.12031100	-2.15045900
C	-4.64068200	-0.28435000	-1.23055600
H	-0.04150700	5.07916000	3.23439600
H	-6.13260500	-0.64922700	-2.72357900
C	-4.14761000	3.24585000	0.34243200
C	-5.20912900	3.27949800	1.49514500
H	-5.23591700	2.29482600	1.97636800
H	-6.21623200	3.49771400	1.12783800
H	-6.54353400	4.18127000	-1.14343800
H	-5.51822100	4.34457500	-2.56435900
C	-1.54089800	3.20819500	0.84761900
H	-2.39832300	5.39211300	3.93946300
H	-6.67283300	1.73998900	-3.11166800
C	-4.67433400	4.33103200	2.48855200
H	-4.97336600	4.12662000	3.52298800
H	-5.04507700	5.33698700	2.24759700
C	-5.55877400	3.91986000	-1.55493600
C	-4.41535000	4.42608300	-0.65062700
H	-3.51290200	4.59304500	-1.24966900
H	-4.65008300	5.36094900	-0.13284900
C	-4.45031000	-1.75579500	-1.03116600
C	-4.01791700	-2.56597700	-2.11084700
C	-4.89801400	-2.35644300	0.17410300
C	-3.54538500	-2.02013900	-3.34774800
C	-4.04888700	-4.00608000	-1.98196800
C	-4.87232700	-3.79706800	0.30491900
C	-3.18201100	-2.83222600	-4.39089900
H	-3.44238200	-0.94649700	-3.44314500
C	-3.66773500	-4.81640400	-3.09671800
C	-4.45530300	-4.57941600	-0.77495400
C	-3.25876000	-4.24911000	-4.27360400
H	-2.80527700	-2.38867000	-5.30741000
H	-3.70808200	-5.89713300	-2.98404300
H	-4.46465000	-5.66322200	-0.67914500
H	-2.97216700	-4.87486700	-5.11448300
C	0.95489500	3.67187800	1.21542000
C	1.86298500	3.11280700	2.14942300
C	1.42937400	4.21366100	-0.00548700
C	1.45774300	2.58143700	3.41760700
C	3.27326800	3.07632900	1.83536200
C	2.83448900	4.11487600	-0.32865200
C	2.37468900	2.10870000	4.32010300
H	0.40283000	2.56294900	3.66612100
C	4.19478600	2.56418800	2.80113100

C	3. 71548100	3. 54918500	0. 59703800
C	3. 76504600	2. 10597000	4. 01598700
H	2. 03830200	1. 71761100	5. 27638600
H	5. 25111700	2. 54965300	2. 54448000
H	4. 77105200	3. 47851600	0. 34900500
H	4. 47459700	1. 72083500	4. 74219000
C	-5. 88296100	-2. 22493800	2. 41070200
H	-6. 29914200	-1. 62847000	3. 21838500
C	-5. 43966400	-1. 60809400	1. 26910900
H	-5. 51332200	-0. 53009700	1. 18285100
C	-5. 81204500	-3. 64026100	2. 54999200
H	-6. 16166700	-4. 11103200	3. 46475600
C	-5. 32145500	-4. 39926100	1. 52232600
H	-5. 27948100	-5. 48290900	1. 60361000
C	1. 07662600	5. 38061800	-2. 12384400
H	0. 41058300	5. 89029000	-2. 81506600
C	2. 45224000	5. 23117400	-2. 45954900
H	2. 81984100	5. 61203600	-3. 40840900
C	3. 30453900	4. 61722800	-1. 58279000
H	4. 35692200	4. 49212500	-1. 82163000
C	0. 58399400	4. 88863700	-0. 94359700
H	-0. 46602400	5. 01911500	-0. 70746000
C	-1. 25315400	-1. 91438300	3. 76824500
C	-1. 27830900	-3. 03659600	2. 68478000
H	-1. 63985200	-3. 99064600	3. 08161300
H	-1. 95892000	-2. 75712800	1. 87722400
C	0. 23787600	-3. 74464900	0. 71312500
C	-0. 58399600	-3. 22984000	-0. 30047000
C	1. 12090100	-4. 78110500	0. 36678000
C	-0. 51633600	-3. 71326900	-1. 60611700
H	-1. 29231400	-2. 43617200	-0. 08541400
C	1. 18244000	-5. 27755000	-0. 93580900
H	1. 77284700	-5. 22207600	1. 11049300
C	0. 36693300	-4. 74217200	-1. 92968600
H	-1. 14296400	-3. 27386100	-2. 37305800
H	1. 87702700	-6. 08066200	-1. 16800400
H	0. 41845000	-5. 11611200	-2. 94827100
C	0. 16429000	-3. 19719900	2. 14318200
C	0. 11802900	-1. 22043900	3. 54035800
H	0. 83737400	-1. 47325100	4. 32147700
H	0. 04857500	-0. 13105900	3. 49774100
N	0. 62915000	-1. 70555800	2. 21489200
C	2. 06991300	-1. 51371300	2. 02317700
N	2. 38250800	-1. 40431500	0. 71360600

C	3.68779200	-1.23484900	0.16844900
C	4.71880700	-2.13461700	0.44871600
C	3.90503100	-0.17311100	-0.71281100
C	5.96612100	-1.96068000	-0.14884500
C	5.15652400	-0.01601200	-1.31035800
H	3.10033400	0.51377400	-0.93768100
C	6.19444200	-0.90341800	-1.03091300
H	7.16545900	-0.77815300	-1.49571500
C	5.40724700	1.15268400	-2.22688000
C	7.05738700	-2.96919800	0.09775300
F	4.27754900	1.59200300	-2.81437100
F	6.28732600	0.84246800	-3.20301100
F	5.93880400	2.21177200	-1.55517600
F	8.28322200	-2.40345700	0.03593400
F	7.03631000	-3.95989500	-0.82470500
F	6.93816700	-3.55603000	1.30745700
S	3.17308400	-1.44002800	3.26770900
H	4.54973200	-2.96042300	1.12665500
H	1.63237700	-1.31735000	0.02476300
H	-0.10020100	-0.67965200	1.30343500
C	0.98145100	-4.06682800	3.11759300
H	0.94511500	-3.67947300	4.13474900
H	2.03532300	-4.13268300	2.84491300
H	0.56031200	-5.07709300	3.12516200
N	-1.25980400	0.21473900	-1.66765100
S	0.00071700	-0.18732400	-2.56411700
O	-0.45342400	-0.83665300	-3.79012600
O	1.08628800	-0.81353100	-1.78255900
C	0.74621200	1.43957300	-3.10761900
F	-0.18894400	2.25611200	-3.59437400
F	1.66803300	1.21258200	-4.04390000
F	1.33056000	2.02085100	-2.05017400
C	-2.42051300	-0.93099200	3.57143100
H	-3.38069500	-1.44968500	3.66338400
H	-2.38950100	-0.14047700	4.33204700
H	-2.39615700	-0.45487300	2.58924000
C	-1.35052100	-2.47266300	5.20245500
H	-1.24946500	-1.66543100	5.93838400
H	-2.32725200	-2.94451200	5.36216600
H	-0.58076900	-3.21853200	5.42196700

TS-1-1-IS

l imaginary frequencies

H = -5198.724532

G = -5198.915476

E(M06-2X-DCM) = -5199.558744

C	0.64177300	-2.25497400	-4.28725900
C	0.44492600	-0.83025800	-4.93565800
H	1.40984400	-0.56310600	-5.37768800
H	-0.25534900	-0.95640600	-5.76689800
C	-1.43218500	0.57514700	-3.86687400
C	-2.41782400	0.06342300	-4.74195900
C	-1.86349100	1.35880100	-2.77039600
C	-3.76635500	0.32880700	-4.53539200
H	-2.13566600	-0.52421500	-5.60705100
C	-3.21393300	1.59329200	-2.54933200
H	-1.13936000	1.74819900	-2.06358400
C	-4.16961800	1.08621900	-3.43516400
H	-4.50323500	-0.07091200	-5.22491600
H	-3.52339500	2.17163300	-1.68561900
H	-5.22528400	1.27507900	-3.26228700
C	-0.00717500	0.33306000	-4.08620000
C	-0.65287300	-2.85062100	-3.68607100
H	-0.47715500	-3.91888500	-3.49191600
H	-1.46999600	-2.80101100	-4.41153300
N	-1.09400900	-2.19878500	-2.46643800
C	-2.33681700	-2.35039000	-1.92833800
N	-2.43883500	-1.68008800	-0.72886500
C	-3.46684600	-1.50979000	0.20180000
C	-4.74547700	-2.08408100	0.14142500
C	-3.14825600	-0.67925100	1.29657100
C	-5.66758400	-1.81976800	1.15782200
C	-4.08101700	-0.43356100	2.29573100
H	-2.16671400	-0.21928200	1.35065600
C	-5.35727000	-1.00012900	2.24002700
H	-6.08701800	-0.80577800	3.01654600
C	-3.70056400	0.41503400	3.47780300
C	-7.05848200	-2.38798400	1.03443400
F	-3.32055200	-0.33089900	4.54362200
F	-4.72709300	1.19175100	3.89291200
F	-2.66360900	1.24476200	3.19870800
F	-7.66485600	-2.50101200	2.23827500
F	-7.05715700	-3.61059100	0.46459300
F	-7.84970100	-1.59790900	0.27011600
S	-3.55141800	-3.24668500	-2.68184700
C	1.04541000	-3.18714000	-5.45126500
H	1.93913300	-2.81200400	-5.96225100
H	1.27209200	-4.19079400	-5.07594600

H	0.24282700	-3.27873900	-6.19312600
C	1.79074900	-2.22813200	-3.26466700
H	1.95985000	-3.22990600	-2.85559900
H	2.72247900	-1.89929000	-3.73896100
H	1.60626900	-1.55784100	-2.42252000
H	-5.00625400	-2.72592500	-0.68834400
C	0.96901700	1.20593600	-3.56568500
H	-1.58353400	-1.19203900	-0.45647900
H	1.94548400	1.17142300	-4.04969700
H	0.64678500	2.22014800	-3.32970600
H	-0.37702500	-1.81678400	-1.85418000
H	1.40710900	0.88486800	-2.37869900
O	0.37937100	1.50717000	0.92234700
O	2.29798200	-0.25571400	1.20751000
P	1.20032400	0.32136600	0.15786500
O	0.16954500	-0.65748100	-0.29647600
C	2.44279900	4.73073200	2.63541200
C	2.43869100	3.48669800	3.25567700
C	1.66652000	2.43372700	2.74296600
C	0.90726600	3.87931900	0.92931400
C	1.64190700	4.92642300	1.51290300
C	1.82439300	-0.92695200	2.35459700
C	1.39797300	-0.16661900	3.44012500
C	0.75311600	-0.80707200	4.51004400
C	0.63936400	-2.19253900	4.54147800
C	1.18982700	-2.94039700	3.50192000
C	1.78294000	-2.33415900	2.38090200
H	1.58264100	5.90967900	1.05614200
H	1.15017600	-4.02507600	3.53521100
C	1.60680600	1.30564800	3.76813200
C	2.97172400	1.52242400	4.50278400
H	2.97807000	1.08028200	5.50403900
H	3.76601400	1.04454800	3.91810600
H	-0.79306700	0.01813200	5.79572700
H	0.84201200	0.17389200	6.44142100
C	1.00197300	2.60953100	1.53032400
H	3.03632000	5.54991200	3.03285500
H	0.14337500	-2.69118300	5.37013200
C	3.17477400	3.05284000	4.50431700
H	2.74185800	3.51575900	5.40200100
H	4.23298000	3.33675200	4.48308400
C	0.25013500	0.20358500	5.51621600
C	0.42185600	1.54240700	4.76658600
H	0.60476600	2.39240200	5.43073700

H	-0.48648200	1.75384200	4.19487400
C	2.39268700	-3.21233800	1.33243400
C	3.80397200	-3.31975100	1.25486100
C	1.57063600	-4.03265800	0.52287600
C	4.68812000	-2.60174800	2.12236600
C	4.39891700	-4.22560900	0.29830500
C	2.18057900	-4.96003000	-0.40482100
C	6.04838000	-2.73939700	2.02995600
H	4.26617100	-1.93954300	2.86985600
C	5.82329400	-4.32460700	0.22024700
C	3.57314900	-5.01563600	-0.50588400
C	6.62909200	-3.60303000	1.05877800
H	6.69392100	-2.18217800	2.70340800
H	6.25170000	-5.00111100	-0.51560600
H	4.02683700	-5.71018400	-1.21034300
H	7.71005700	-3.69246000	0.99476100
C	0.00249900	4.21782300	-0.21698100
C	-1.40265200	4.24078100	-0.01288000
C	0.54796400	4.67882800	-1.44163100
C	-2.02547700	3.79713100	1.19863800
C	-2.26577300	4.76038600	-1.05122400
C	-0.33123700	5.17495100	-2.47835500
C	-3.38484300	3.84839100	1.36918400
H	-1.40501700	3.41055300	1.99762100
C	-3.67822800	4.81237500	-0.82791400
C	-1.70928800	5.20938400	-2.25177400
C	-4.22689300	4.36733700	0.34490400
H	-3.82477400	3.48401300	2.29239100
H	-4.30749400	5.21571100	-1.61805400
H	-2.36534500	5.59940900	-3.02743900
H	-5.30130800	4.41088400	0.50137900
C	-0.62697100	-4.84458600	-0.17777600
H	-1.71003700	-4.80216700	-0.11301000
C	0.13958500	-4.00370700	0.58677200
H	-0.33827200	-3.29615600	1.25404200
C	-0.01986600	-5.76706200	-1.07795600
H	-0.64688800	-6.42577200	-1.67223800
C	1.34386500	-5.81414100	-1.19116700
H	1.82124500	-6.51286100	-1.87467800
C	2.45192100	5.10876800	-2.91264200
H	3.52114300	5.06347900	-3.09577900
C	1.58231800	5.60175800	-3.92635500
H	1.99647600	5.94899200	-4.86910700
C	0.23053400	5.63175500	-3.71213100

H	-0.44611800	6.00466800	-4.47757400
C	1.95468000	4.66971600	-1.71274600
H	2.63336700	4.29030800	-0.95854100
N	2.09228600	0.87784000	-1.10677000
S	3.61793600	1.46694800	-1.15892600
C	4.74837400	-0.03064100	-0.93283100
O	3.93643000	2.34929000	-0.03483800
O	3.85311400	1.89900600	-2.53872500
F	5.07775500	-0.16481500	0.34728400
F	4.15077000	-1.14783100	-1.36316600
F	5.85466100	0.17536100	-1.65135100

TS-1-1-1S-1

1 imaginary frequencies

H = -5198.720781

G = -5198.912014

E(M06-2X-DCM) = -5199.557055

C	0.23760200	-2.24838700	-4.33471100
C	0.25692100	-0.77211300	-4.89318900
H	1.24758900	-0.63295800	-5.33661800
H	-0.46072200	-0.73819400	-5.71965500
C	-1.37817200	0.82545600	-3.69837500
C	-2.45252600	0.49442500	-4.55466300
C	-1.66060400	1.60853600	-2.55516500
C	-3.74381600	0.93334900	-4.28533800
H	-2.28253500	-0.08760000	-5.45237600
C	-2.95685400	2.01859900	-2.27317900
H	-0.86698900	1.86130400	-1.86151500
C	-4.00212600	1.68953100	-3.14146100
H	-4.55130700	0.66910000	-4.96081900
H	-3.15305200	2.59477100	-1.37551900
H	-5.01505800	2.01425000	-2.92129100
C	-0.00507100	0.40782300	-3.98609800
C	-1.12654600	-2.68887100	-3.75238100
H	-1.10474500	-3.78145400	-3.62727000
H	-1.93415400	-2.47728300	-4.45926400
N	-1.45754900	-2.06019000	-2.48696400
C	-2.70204600	-2.04897100	-1.93776400
N	-2.69160800	-1.42404500	-0.70771400
C	-3.68693800	-1.08189100	0.21000100
C	-5.03127400	-1.48259000	0.16185500
C	-3.26204100	-0.26618900	1.27899100
C	-5.91161000	-1.06162500	1.16145700
C	-4.15591800	0.13674300	2.26366900

H	-2.22774000	0.06054500	1.32353600
C	-5.49625700	-0.25411000	2.21799600
H	-6.19479200	0.06286300	2.98252000
C	-3.66200000	0.96138900	3.42016800
C	-7.36613700	-1.44195200	1.05025800
F	-3.28684800	0.19255400	4.47247100
F	-4.60543500	1.81336900	3.87663100
F	-2.57830000	1.71039200	3.08714900
F	-7.97751300	-1.44982900	2.25708900
F	-7.53011100	-2.66441400	0.50465400
F	-8.04806200	-0.56787700	0.27222500
S	-4.04486400	-2.71803200	-2.70946000
C	0.49346000	-3.15392600	-5.56037600
H	1.43141000	-2.88394400	-6.05813200
H	0.56998000	-4.20191200	-5.25151100
H	-0.31650100	-3.07822200	-6.29618900
C	1.38230900	-2.45685700	-3.32875500
H	1.40154300	-3.49452200	-2.97906200
H	2.35223000	-2.24343200	-3.79103700
H	1.30248800	-1.82025700	-2.44522000
H	-5.37388100	-2.11135900	-0.64789500
C	1.08976600	1.14046000	-3.49160000
H	-1.77193700	-1.07639800	-0.43233800
H	2.04037300	0.98372700	-4.00159600
H	0.90453000	2.18108100	-3.22771500
H	-0.68598700	-1.79418100	-1.88041600
H	1.53185100	0.76042900	-2.30331700
O	0.58048600	1.36072500	0.85100100
O	2.20553200	-0.66059000	1.19589300
P	1.22232500	0.04524700	0.12257300
O	0.05824500	-0.76964300	-0.33177400
C	3.13438100	4.18966000	2.60455200
C	2.89155100	2.97510100	3.23511400
C	1.96349500	2.06206700	2.70740500
C	1.52348100	3.59753000	0.86017500
C	2.41616900	4.50637700	1.45378400
C	1.61570000	-1.27189200	2.31999400
C	1.28240100	-0.46318600	3.39987300
C	0.53511300	-1.00638000	4.45492400
C	0.22735900	-2.36330900	4.47160600
C	0.68173400	-3.17709800	3.43346500
C	1.37303900	-2.65666200	2.32473900
H	2.54465300	5.47769500	0.98570600
H	0.48569100	-4.24479000	3.45888300

C	1. 70246000	0. 96005600	3. 73389900
C	3. 07150600	0. 96018400	4. 49315400
H	2. 99452900	0. 51508600	5. 48982700
H	3. 79134600	0. 37034200	3. 91360600
H	-0. 89126000	0. 03998900	5. 72193100
H	0. 73990200	-0. 04677500	6. 38920000
C	1. 37195100	2. 33796900	1. 47321500
H	3. 85029900	4. 89709500	3. 01496900
H	-0. 34646300	-2. 79296400	5. 28862100
C	3. 50843700	2. 43905900	4. 50807200
H	3. 11777600	2. 96568900	5. 38979900
H	4. 59767100	2. 55862400	4. 52770000
C	0. 17097000	0. 06785400	5. 45621600
C	0. 54751000	1. 36881400	4. 71107400
H	0. 83876300	2. 18382500	5. 38061000
H	-0. 31119900	1. 70856200	4. 12387000
C	1. 86298600	-3. 58295000	1. 25745900
C	3. 25588900	-3. 80214700	1. 11100900
C	0. 93853100	-4. 30828400	0. 46641400
C	4. 23945100	-3. 14677600	1. 91861600
C	3. 72748800	-4. 75305100	0. 13071000
C	1. 42623500	-5. 27615200	-0. 49120600
C	5. 57801700	-3. 38475500	1. 74969300
H	3. 91356000	-2. 45360200	2. 68546700
C	5. 13296000	-4. 96721600	-0. 01914800
C	2. 80294400	-5. 46448200	-0. 63776800
C	6. 03684400	-4. 30137200	0. 76242100
H	6. 30042600	-2. 87020200	2. 37774800
H	5. 46640300	-5. 67897400	-0. 77062700
H	3. 16457600	-6. 19006900	-1. 36384700
H	7. 10272300	-4. 47253500	0. 63920600
C	0. 71657600	4. 08713100	-0. 30494700
C	-0. 65432500	4. 40265600	-0. 11042900
C	1. 35107500	4. 40884700	-1. 53028500
C	-1. 36330800	4. 09982400	1. 09709000
C	-1. 38467200	5. 08452800	-1. 15648800
C	0. 60124700	5. 07422500	-2. 57386800
C	-2. 68353000	4. 43336700	1. 25803000
H	-0. 84332800	3. 59207600	1. 90010100
C	-2. 75592300	5. 43138100	-0. 94235100
C	-0. 73916400	5. 40141700	-2. 35474000
C	-3. 39195700	5. 11586400	0. 22833800
H	-3. 19457200	4. 16807700	2. 17856800
H	-3. 28343200	5. 95163700	-1. 73839100

H	-1.29411700	5.91743900	-3.13560600
H	-4.43447700	5.38329700	0.37767600
C	-1.34732700	-4.86263300	-0.20696500
H	-2.41756800	-4.69842100	-0.12336400
C	-0.47995500	-4.12769500	0.55945600
H	-0.86854300	-3.38374900	1.24497400
C	-0.86093500	-5.83012400	-1.13236300
H	-1.56560300	-6.40463200	-1.72704900
C	0.48743700	-6.02370500	-1.27055500
H	0.87428900	-6.75583200	-1.97601800
C	3.30546300	4.40436800	-2.99895000
H	4.33978400	4.12745700	-3.18045300
C	2.56558900	5.07023000	-4.01750600
H	3.04719500	5.31421200	-4.96046200
C	1.25190600	5.39231100	-3.80794400
H	0.67337100	5.89697100	-4.57817900
C	2.72199900	4.09070200	-1.79891200
H	3.29481200	3.56851800	-1.04460400
N	2.23656400	0.56413800	-1.07312400
S	3.76692800	0.04128000	-1.39976500
C	4.86907400	0.79354000	-0.05725200
O	4.16859100	0.72346000	-2.63290400
O	3.94405100	-1.40327200	-1.26660600
F	4.43457900	2.00931500	0.30158000
F	4.91623300	0.01890000	1.02455300
F	6.09626300	0.90537100	-0.56850700

TS-1-1-1R

1 imaginary frequencies

H = -5198.716238

G = -5198.905118

E(M06-2X-DCM) = -5199.552514

C	1.06418900	3.31537800	3.74253600
C	-0.13017200	2.64295500	4.52714100
H	-0.96120900	3.35375500	4.49126200
H	0.17796400	2.57098200	5.57411900
C	0.03878300	0.08272000	4.55365400
C	0.78162900	0.07218800	5.75697500
C	-0.06427400	-1.12550100	3.82585500
C	1.38316800	-1.09408300	6.21702400
H	0.86229900	0.96588700	6.36422200
C	0.56887500	-2.27736100	4.27336900
H	-0.57893900	-1.14139300	2.87146000
C	1.28652600	-2.27001300	5.47300600

H	1. 93575300	-1. 08041100	7. 15171000
H	0. 50227700	-3. 18155500	3. 67955100
H	1. 77442500	-3. 17596900	5. 82151300
C	-0. 62996000	1. 29450800	4. 07876500
C	2. 26981800	2. 37876700	3. 50687100
H	3. 13179200	2. 99476400	3. 21331500
H	2. 55804900	1. 87730200	4. 43519800
N	2. 03768000	1. 35131100	2. 49986500
C	2. 93911800	0. 34916100	2. 24375300
N	2. 49698800	-0. 48173500	1. 23995400
C	3. 15706100	-1. 42715300	0. 44221200
C	4. 52682600	-1. 72774900	0. 49366400
C	2. 35729200	-2. 08047900	-0. 51403100
C	5. 06562400	-2. 64641500	-0. 40904300
C	2. 91703500	-2. 99101700	-1. 40310300
H	1. 29812000	-1. 85426200	-0. 56096100
C	4. 27998800	-3. 28876000	-1. 36440200
H	4. 71417100	-4. 00316100	-2. 05283400
C	2. 04896200	-3. 57962600	-2. 47941000
C	6. 55332600	-2. 87826300	-0. 40656400
F	0. 78451800	-3. 80994100	-2. 05316000
F	1. 94269800	-2. 74357400	-3. 54992100
F	2. 53495800	-4. 74736600	-2. 95024500
F	6. 87444100	-4. 10949600	-0. 86409600
F	7. 19250300	-1. 98837400	-1. 21250700
F	7. 09249100	-2. 74684600	0. 82143400
S	4. 36103900	0. 18725600	3. 12692300
C	1. 56929500	4. 46213000	4. 64520200
H	0. 74503900	5. 12728600	4. 92621200
H	2. 31830500	5. 06375700	4. 11932500
H	2. 02769700	4. 08000400	5. 56565400
C	0. 55700900	3. 92523400	2. 42644700
H	1. 37831500	4. 41223900	1. 89239200
H	-0. 21172500	4. 68005900	2. 61875900
H	0. 09957000	3. 19594800	1. 75373500
H	5. 15648800	-1. 25106500	1. 23067500
C	-1. 76578300	1. 23553300	3. 24963600
H	1. 50150500	-0. 40257800	1. 01028700
H	-2. 41520900	2. 11134600	3. 30045900
H	-2. 30082000	0. 28779400	3. 20736500
H	1. 41700200	1. 60061800	1. 73920700
H	-1. 50361900	1. 40763500	1. 97017900
O	-2. 49943900	-0. 29672700	-0. 93536000
O	-0. 15327300	0. 65771500	-1. 56744400

P	-1.12327900	0.30060600	-0.31429100
O	-0.35043500	-0.62151900	0.56838400
C	-2.32299000	-3.89761000	-3.08821500
C	-1.99361000	-2.69174200	-3.69397900
C	-2.13223500	-1.47728200	-3.00142500
C	-2.84125500	-2.70776700	-1.01301100
C	-2.77397700	-3.89000000	-1.77102900
C	-0.46304600	1.48877800	-2.65570300
C	-1.39009900	1.06872000	-3.60705600
C	-1.83931900	1.99151000	-4.56538700
C	-1.25685900	3.24905400	-4.66820100
C	-0.19723400	3.57154900	-3.82371000
C	0.22184400	2.71280700	-2.79281700
H	-3.05570400	-4.82210400	-1.29108500
H	0.32096100	4.51752400	-3.94517100
C	-1.92927400	-0.31430800	-3.96515500
C	-0.97330900	-0.99399800	-5.00707300
H	-0.97409000	-0.47977300	-5.97239900
H	0.04868100	-0.96998700	-4.61222700
H	-2.60652200	1.19876700	-6.43432500
H	-3.81210700	2.06163400	-5.48573600
C	-2.48618000	-1.50543600	-1.65569900
H	-2.22929300	-4.83574600	-3.62884600
H	-1.59322500	3.95912400	-5.41928700
C	-1.44871800	-2.45822800	-5.08400400
H	-0.63395200	-3.14912900	-5.32727100
H	-2.22553000	-2.59516200	-5.84902000
C	-2.94584300	1.39474900	-5.40779600
C	-3.27268600	0.08429400	-4.65995400
H	-4.02384000	0.27538000	-3.88481400
H	-3.65621200	-0.70614300	-5.31241300
C	1.42029900	3.09744000	-1.98411800
C	1.43589200	4.32342100	-1.26992000
C	2.59851800	2.30699800	-2.06237600
C	0.27868600	5.15873900	-1.13018100
C	2.66180100	4.77207000	-0.64632200
C	3.79636500	2.73923200	-1.37708800
C	0.34411300	6.36460000	-0.47990600
H	-0.66789400	4.81738100	-1.53186000
C	2.68775500	6.04166900	0.01386600
C	3.79838200	3.96137600	-0.69947900
C	1.56683800	6.82450500	0.08620900
H	-0.55165200	6.97236900	-0.38674400
H	3.62575500	6.37082900	0.45552300

H	4.71283200	4.29525500	-0.21314600
H	1.60117900	7.78907000	0.58579500
C	-3.30634800	-2.80989100	0.40491300
C	-2.55796800	-3.58465900	1.32755000
C	-4.56026000	-2.26856700	0.78379900
C	-1.29138300	-4.17513300	1.00457800
C	-3.08743100	-3.82475000	2.65185300
C	-5.04447700	-2.46285100	2.13229600
C	-0.64711000	-5.00497200	1.88618800
H	-0.83989700	-3.96627500	0.04228400
C	-2.37728600	-4.68788800	3.54450900
C	-4.29762300	-3.23471400	3.02646000
C	-1.20353500	-5.28284200	3.16821500
H	0.30303300	-5.45216200	1.60633900
H	-2.80312900	-4.87202700	4.52803700
H	-4.68458800	-3.40824400	4.02867100
H	-0.68440600	-5.95362400	3.84774000
C	3.83275400	0.35274300	-2.86565600
H	3.85093100	-0.56754700	-3.44206500
C	2.68441000	1.09937900	-2.82729800
H	1.82234500	0.77273000	-3.39570600
C	4.99171600	0.75684400	-2.14453900
H	5.87938300	0.13183700	-2.15583400
C	4.97039200	1.92346600	-1.42957700
H	5.84999500	2.25536500	-0.88350300
C	-6.62486200	-1.06731400	0.26631900
H	-7.25007200	-0.54202900	-0.45051900
C	-7.07564100	-1.22264800	1.60760900
H	-8.03576800	-0.80969800	1.90470300
C	-6.30537200	-1.90374400	2.51060800
H	-6.64546200	-2.04839300	3.53339000
C	-5.41327000	-1.57057700	-0.12930000
H	-5.09036000	-1.44428500	-1.15595100
N	-1.62281600	1.61579200	0.55818700
S	-2.67962100	2.81307900	0.19195700
C	-4.39212300	2.05146900	0.37545000
O	-2.61011100	3.78149600	1.28837700
O	-2.60209500	3.24281900	-1.20438500
F	-5.26069200	3.03162000	0.63503200
F	-4.39829200	1.18211900	1.39384300
F	-4.75917300	1.43407000	-0.74612900

TS-1-1-1R-1

1 imaginary frequencies

H = -5198.708876

G = -5198.898736

E(M06-2X-DCM) = -5199.543815

C	-0.25683900	3.08571700	3.88850100
C	-0.98673000	1.94756300	4.70139000
H	-2.02797700	2.26761000	4.80702000
H	-0.55985600	1.94641400	5.70832300
C	0.15979400	-0.33654800	4.44502400
C	1.04582500	-0.07356600	5.51721000
C	0.39275700	-1.49474900	3.66594400
C	2.10865700	-0.92449400	5.79559300
H	0.89410600	0.78339200	6.16176700
C	1.47203800	-2.32712300	3.93158800
H	-0.23229200	-1.70255100	2.80702600
C	2.33018900	-2.04923400	4.99947100
H	2.76863000	-0.70422800	6.62917600
H	1.64722700	-3.19262700	3.30226700
H	3.17079900	-2.70555900	5.20670200
C	-0.97763100	0.53923400	4.16064200
C	1.22162200	2.78759300	3.55471100
H	1.69895000	3.72884700	3.25451800
H	1.75582400	2.45557300	4.45291400
N	1.42895400	1.80837000	2.49739400
C	2.66718200	1.43780900	2.06554600
N	2.60224400	0.48689000	1.07273600
C	3.57191000	-0.06209000	0.22633200
C	4.90950600	0.35250100	0.13544100
C	3.12353500	-1.08954400	-0.62629100
C	5.75583100	-0.24638900	-0.79919000
C	3.98687600	-1.67457900	-1.54605200
H	2.08970600	-1.41302700	-0.56980800
C	5.31660300	-1.26048200	-1.64674900
H	5.98649400	-1.71104900	-2.36894400
C	3.50125000	-2.79837800	-2.41828900
C	7.15132900	0.29385500	-0.96456900
F	3.77233900	-4.01553100	-1.87625800
F	2.16203500	-2.75556500	-2.61531300
F	4.08693200	-2.78358900	-3.63535700
F	8.00591800	-0.64456900	-1.43056400
F	7.17908400	1.31899200	-1.85891600
F	7.65882900	0.77072700	0.18857400
S	4.06551600	2.09195400	2.74587500
C	-0.24523400	4.31759300	4.82156100
H	-1.25647300	4.54786200	5.17550900

H	0.13100700	5.19760500	4.28941000
H	0.39249600	4.15352600	5.69870300
C	-1.05991500	3.44509100	2.62953600
H	-0.57169700	4.26215400	2.09135300
H	-2.06666300	3.77975400	2.90068200
H	-1.18099600	2.61379400	1.93087600
H	5.27439400	1.13439600	0.78536800
C	-2.09546100	0.10387800	3.42733600
H	1.66336200	0.12545900	0.88404600
H	-3.02782900	0.62851400	3.64097900
H	-2.23177100	-0.96991200	3.30821800
H	0.62601000	1.43860900	2.00241500
H	-2.11273700	0.46053000	2.14498300
O	-2.14055900	-1.43438000	-0.68486700
O	-0.73436000	0.63954300	-1.41705200
P	-1.30704600	-0.17477200	-0.13365700
O	-0.11797800	-0.47328600	0.72098800
C	-0.92149000	-4.23778700	-3.53589300
C	-1.30604800	-2.96096300	-3.92701100
C	-1.77803400	-2.02564900	-2.98934100
C	-1.39188300	-3.66295200	-1.20678400
C	-1.00018100	-4.58706300	-2.19040100
C	-1.50237700	1.33874400	-2.35693200
C	-2.33943200	0.64165800	-3.22344600
C	-3.29261800	1.36220400	-3.96233700
C	-3.25212800	2.75130400	-3.99913300
C	-2.24597300	3.41885800	-3.29964200
C	-1.36136700	2.74253300	-2.44089700
H	-0.73656900	-5.59211900	-1.87643000
H	-2.14671000	4.49546000	-3.39624300
C	-2.33614100	-0.80453700	-3.72083300
C	-1.47511800	-0.86922100	-5.03454100
H	-1.93353800	-0.31890400	-5.86053300
H	-0.49713900	-0.41543500	-4.83536000
H	-4.12277300	0.45211000	-5.75441000
H	-5.29189100	0.66593100	-4.45645500
C	-1.74006000	-2.36755000	-1.63945500
H	-0.57276500	-4.96055700	-4.26881400
H	-3.96717500	3.31348700	-4.59445400
C	-1.29841800	-2.37179400	-5.31760100
H	-0.37447200	-2.59626300	-5.86228700
H	-2.12669600	-2.76702300	-5.92220500
C	-4.24516300	0.41566700	-4.66341300
C	-3.84742500	-0.96428200	-4.08634400

H	-4.41103200	-1.15999900	-3.16855900
H	-4.02454600	-1.79023900	-4.78203800
C	-0.26502900	3.50075300	-1.75712700
C	-0.56132400	4.61122300	-0.92165900
C	1.09034100	3.17583000	-2.04199600
C	-1.89662900	5.02054400	-0.60048800
C	0.51827600	5.38574500	-0.34834500
C	2.15458300	3.93353400	-1.42209000
C	-2.14571900	6.12085000	0.17925400
H	-2.72658300	4.44186400	-0.97908200
C	0.21602900	6.52483200	0.46362400
C	1.84098300	5.01324100	-0.59420600
C	-1.07791500	6.89409900	0.71494400
H	-3.17257200	6.40111600	0.39889700
H	1.04663800	7.09651200	0.87120800
H	2.64807000	5.58595700	-0.14249500
H	-1.29411500	7.76666200	1.32545500
C	-1.45232100	-4.11413700	0.21880200
C	-0.27916800	-4.61930300	0.83851300
C	-2.69153200	-4.14959400	0.90991500
C	1.01298600	-4.57439900	0.21929800
C	-0.36269300	-5.20767400	2.15697400
C	-2.74482500	-4.68891900	2.25128000
C	2.11898900	-5.11337000	0.82497900
H	1.11619100	-4.10329800	-0.75006000
C	0.81122000	-5.77425200	2.74751700
C	-1.58648700	-5.21374200	2.83049800
C	2.01750200	-5.73971000	2.09997000
H	3.08040900	-5.05427100	0.32489000
H	0.72027400	-6.23343700	3.72928700
H	-1.64166000	-5.64646700	3.82751500
H	2.90050200	-6.17819300	2.55730500
C	2.79627500	1.85448000	-3.19820700
H	3.05295000	1.06489100	-3.89924100
C	1.47835800	2.14542000	-2.95843300
H	0.71065700	1.59322600	-3.48670700
C	3.83672500	2.56991700	-2.54150100
H	4.87439500	2.30272600	-2.71523200
C	3.51689200	3.58575800	-1.68325000
H	4.29544100	4.15288800	-1.17955500
C	-5.09655700	-3.72683700	1.04141700
H	-6.00885400	-3.35927600	0.58096200
C	-5.13482200	-4.22871000	2.37276800
H	-6.07465300	-4.23916400	2.91768200

C	-3.99073600	-4.70253000	2.95408800
H	-4.00536100	-5.10495200	3.96433900
C	-3.92283200	-3.69730300	0.33478800
H	-3.92633500	-3.31670800	-0.67873300
N	-2.46074800	0.62121600	0.76379800
S	-4.10464100	0.55359500	0.58273400
C	-4.57670800	2.34663300	0.34444400
O	-4.55903200	-0.09996400	-0.64344700
O	-4.69313000	0.20402500	1.87751600
F	-5.89611200	2.45356100	0.51520700
F	-4.26803100	2.74455600	-0.89382800
F	-3.95881600	3.13554300	1.23018700

TS-1-2-2S

l imaginary frequencies

H = -5198.715898

G = -5198.909190

E(M06-2X-DCM) = -5199.556672

O	2.97645400	1.38013200	0.18368000
O	2.90664500	-1.05883800	-0.72741500
P	2.08436300	0.02502700	0.14916500
O	2.02033800	-0.37033800	1.62638600
N	0.70483500	0.31176300	-0.61476700
S	-0.07176100	-0.59039800	-1.68393100
C	0.79653200	-0.34668600	-3.33474200
F	-0.00848600	-0.78410800	-4.30407900
F	1.06928300	0.94759100	-3.54525800
F	1.94176000	-1.03550600	-3.37782700
C	-0.77395500	1.58949100	3.92650000
C	-1.44171700	0.17885100	4.08331300
H	-1.27368300	-0.12016900	5.12852700
H	-2.51120800	0.34695200	3.96098800
C	-2.00424500	-1.73981100	2.45210000
C	-3.37563100	-1.72673800	2.78943100
C	-1.59998000	-2.52676400	1.35089200
C	-4.29596200	-2.47938500	2.06399900
H	-3.72922900	-1.14861900	3.63451700
C	-2.52533000	-3.25024800	0.60899900
H	-0.56460900	-2.53512000	1.03306600
C	-3.87591000	-3.23614300	0.96833500
H	-5.34776600	-2.44948800	2.33212500
H	-2.18647600	-3.80569100	-0.25965300
H	-4.60110500	-3.80008900	0.38836100
C	-1.00611700	-0.99705500	3.23751800

C	-1.00416300	2.21042900	2.49468300
H	-0.03293100	2.45561700	2.05749600
H	-1.56092100	3.14355200	2.59954700
N	-1.68795500	1.39366100	1.49540200
C	-3.03415700	1.42529500	1.26388300
N	-3.37893400	0.81153200	0.08617300
C	-4.62740200	0.40844700	-0.41708700
C	-5.77343500	0.20775800	0.36278000
C	-4.68552700	0.12200000	-1.79308000
C	-6.93967600	-0.27889600	-0.22938800
C	-5.86276200	-0.34916800	-2.36627800
H	-3.80216700	0.26009100	-2.40680100
C	-7.00603700	-0.55736200	-1.59196800
H	-7.92184600	-0.92038500	-2.04121400
C	-5.88594900	-0.70154700	-3.82995000
C	-8.11186000	-0.57101600	0.66821900
F	-5.00849800	0.03602000	-4.54426400
F	-7.11086900	-0.51232000	-4.37068700
F	-5.56598800	-2.00137700	-4.03523000
F	-9.24487200	-0.81112800	-0.02460300
F	-8.36263400	0.44182500	1.52318100
F	-7.87801700	-1.67217400	1.43422700
S	-4.11653900	2.15921500	2.33337100
H	-5.75313500	0.43173300	1.41913900
C	0.31899600	-1.43510000	3.26549100
H	-2.60877400	0.58936800	-0.54893300
H	0.94116300	-1.07396600	4.08124700
H	0.51856100	-2.46627300	2.98186200
O	-1.38773800	0.04100600	-1.90959100
H	-1.09048900	1.04167600	0.74906000
O	-0.01516300	-2.03635100	-1.44563600
H	1.04698300	-0.82257200	2.27249700
C	6.80862700	-2.10376800	0.37829600
C	6.56543000	-0.94675800	-0.35424600
C	5.26661700	-0.63037100	-0.78186400
C	4.41892900	-2.63264500	0.33703100
C	5.74273300	-2.94694200	0.69005800
C	3.22384800	2.07370600	-1.01466200
C	4.18297400	1.58601700	-1.90196200
C	4.28181900	2.16354000	-3.17873900
C	3.53790100	3.29068800	-3.50730800
C	2.69620400	3.84881300	-2.54698700
C	2.50276200	3.25239800	-1.28877000
H	5.92331700	-3.86723200	1.23735100

H	2. 14804300	4. 75845800	-2. 77197000
C	5. 30505300	0. 56269200	-1. 72927000
C	6. 61164200	1. 26900100	-1. 22529100
H	7. 04877400	1. 92713700	-1. 98183100
H	6. 36357500	1. 88388400	-0. 35237400
H	4. 85634500	1. 18436000	-5. 03857600
H	6. 19194800	1. 95247700	-4. 18801800
C	4. 20958700	-1. 44000000	-0. 37860700
H	7. 81568400	-2. 35623300	0. 70026000
H	3. 62088200	3. 74512300	-4. 49123100
C	7. 54475400	0. 11611600	-0. 79966500
H	8. 15667900	-0. 23628100	-1. 64178200
H	8. 24117600	0. 40631200	-0. 00489900
C	5. 25815600	1. 39251200	-4. 04049000
C	5. 49114000	0. 10880400	-3. 21497900
H	6. 46631700	-0. 35485100	-3. 39267400
H	4. 71608000	-0. 62778300	-3. 45449200
C	1. 61133400	3. 94356000	-0. 30432800
C	2. 17276100	4. 52184200	0. 86395100
C	0. 24056900	4. 14428700	-0. 60925600
C	3. 55433900	4. 38973100	1. 21874400
C	1. 33777700	5. 31774100	1. 73678000
C	-0. 57186900	4. 96944800	0. 25722000
C	4. 05994400	4. 95770400	2. 35878500
H	4. 21395600	3. 83166800	0. 56478500
C	1. 90352800	5. 88909100	2. 92024200
C	-0. 00194000	5. 53234300	1. 40203100
C	3. 22443700	5. 71149100	3. 23085300
H	5. 11253300	4. 83617500	2. 60021600
H	1. 25541700	6. 47736000	3. 56575500
H	-0. 61885400	6. 14975800	2. 05203400
H	3. 64239500	6. 15192400	4. 13192600
C	3. 31800800	-3. 57542000	0. 70490900
C	2. 62689000	-4. 28701600	-0. 30731200
C	3. 03077100	-3. 81795200	2. 07167200
C	2. 90003800	-4. 12105200	-1. 70270100
C	1. 61541800	-5. 25088300	0. 06389600
C	2. 03986600	-4. 80969900	2. 42698800
C	2. 20842800	-4. 82291800	-2. 65392800
H	3. 67301600	-3. 42575000	-2. 00836000
C	0. 91310600	-5. 95960300	-0. 96074200
C	1. 35518000	-5. 48998000	1. 41584000
C	1. 19474600	-5. 75080800	-2. 28297700
H	2. 43375200	-4. 67105800	-3. 70590700

H	0.15168300	-6.67572100	-0.66069500
H	0.60494700	-6.22944900	1.68867000
H	0.65404500	-6.29388100	-3.05306100
C	-1.72434100	3.77309100	-2.01470700
H	-2.18329500	3.29581200	-2.87597100
C	-0.39877300	3.55022500	-1.74516100
H	0.17358800	2.89226600	-2.38513100
C	-2.51234000	4.60601300	-1.17100500
H	-3.56214600	4.76636900	-1.39866200
C	-1.94905800	5.18198600	-0.06483000
H	-2.54363100	5.80256200	0.60065200
C	3.38641700	-3.38913800	4.45386100
H	3.88908800	-2.83633200	5.24309700
C	2.43372500	-4.39058300	4.79716300
H	2.22643700	-4.60223200	5.84258100
C	1.77601800	-5.07217400	3.80887300
H	1.03599300	-5.83004400	4.05512400
C	3.67032000	-3.10999900	3.14169300
H	4.38308000	-2.33026100	2.90060900
C	0.73625100	1.60328300	4.24025000
H	1.09295900	2.64014800	4.26050200
H	0.94123800	1.16940200	5.22712200
H	1.33621100	1.07782700	3.49479600
C	-1.46752200	2.49031700	4.97542600
H	-1.28897200	2.11901900	5.99214800
H	-1.06441700	3.50832500	4.92097600
H	-2.54538300	2.54415500	4.79994200

TS-1-2-2S-1

l imaginary frequencies

H = -5198.710220

G = -5198.903587

E(M06-2X-DCM) = -5199.546336

O	3.32394200	-0.59166700	0.15354800
O	2.21005400	1.68509000	0.77095300
P	1.96529800	0.28724800	0.00333200
O	1.87349200	0.45626100	-1.51341800
N	0.68005400	-0.37143300	0.70652000
S	-0.15066100	0.18379100	1.96734300
C	-0.58912600	-1.39851100	2.85393300
F	-1.45776100	-1.10121500	3.82607500
F	-1.16766200	-2.27121400	2.01630800
F	0.49257600	-1.96270800	3.39875200
C	-0.51195900	-2.15464000	-3.61244200

C	-1.34905500	-0.88335400	-3.99433200
H	-1.16458600	-0.70927800	-5.06480000
H	-2.39348100	-1.17519000	-3.88531700
C	-2.24464500	1.13981400	-2.67003400
C	-3.57561200	0.92458600	-3.08917800
C	-2.01538600	2.08596300	-1.64660300
C	-4.62687100	1.63898600	-2.52002700
H	-3.79421500	0.21931600	-3.88206200
C	-3.06957500	2.77570400	-1.06049000
H	-1.01045400	2.25096000	-1.27523100
C	-4.37846000	2.55998900	-1.50088800
H	-5.64507900	1.45536500	-2.84987200
H	-2.86559900	3.47325500	-0.25448700
H	-5.20364600	3.09732900	-1.04205800
C	-1.11584500	0.44175500	-3.30464400
C	-0.72624500	-2.57572700	-2.10828100
H	0.24775900	-2.65227200	-1.61838600
H	-1.18880600	-3.56386400	-2.07500400
N	-1.51972600	-1.67975800	-1.27357700
C	-2.85739400	-1.83191900	-1.03805100
N	-3.31018400	-1.01782600	-0.03229200
C	-4.61413200	-0.77535000	0.43857100
C	-5.76454100	-0.85681800	-0.35428900
C	-4.73364900	-0.34763300	1.77170100
C	-7.00322700	-0.50488700	0.18328400
C	-5.97955400	-0.00782700	2.29214600
H	-3.84940300	-0.28568700	2.39673300
C	-7.12979100	-0.08197700	1.50411000
H	-8.09821200	0.17809600	1.91254000
C	-6.08057000	0.50408900	3.70454600
C	-8.19572100	-0.52738400	-0.73472300
F	-5.11178000	-0.00069300	4.49786100
F	-7.27046900	0.19278400	4.26593600
F	-5.96704200	1.85294500	3.75404200
F	-9.35575000	-0.31299600	-0.07946400
F	-8.30820300	-1.70056200	-1.39106500
F	-8.09498900	0.43861500	-1.68802300
S	-3.81493900	-2.91546300	-1.91167200
H	-5.68972400	-1.18973600	-1.37918400
C	0.14077400	1.05349500	-3.33964700
H	-2.60450000	-0.47594300	0.47073700
H	0.84900700	0.67979900	-4.07620800
H	0.17893800	2.13208800	-3.19843800
O	-1.47133300	0.67602200	1.51064400

H	-0.97452500	-1.13861900	-0.60366900
O	0.57849500	0.97798900	2.95740300
H	0.87385600	0.68897500	-2.25380000
C	5.74172700	3.92626700	0.71630700
C	5.64763900	2.78295100	1.50182600
C	4.45930300	2.03431500	1.55973700
C	3.44307700	3.59004900	-0.03359000
C	4.63595800	4.33013700	-0.02882300
C	3.58685800	-1.22973200	1.37595300
C	3.96191100	-0.46960400	2.47823400
C	3.92612100	-1.06056400	3.75101300
C	3.71097600	-2.42854800	3.88350800
C	3.54400600	-3.20627800	2.73496800
C	3.45416400	-2.62998600	1.45646000
H	4.68603700	5.23146200	-0.63251100
H	3.44904000	-4.28454300	2.82209400
C	4.59417800	0.91572700	2.59279000
C	6.15726400	0.74345900	2.59871100
H	6.51979700	0.27371700	3.51712300
H	6.44162400	0.09687600	1.76020000
H	3.38037200	-0.05155000	5.59936800
H	5.11657300	-0.15004100	5.32716700
C	3.39189500	2.42528000	0.75293000
H	6.66366700	4.50100200	0.68305000
H	3.69826400	-2.89762500	4.86400200
C	6.71620800	2.15823500	2.36727700
H	6.82662000	2.70540000	3.31410900
H	7.70126200	2.15465400	1.88725800
C	4.15118600	-0.01143700	4.82165800
C	4.10712400	1.31563300	4.02217300
H	4.71902800	2.10692600	4.46692400
H	3.07451500	1.67314300	3.95531500
C	3.31924100	-3.49560800	0.24128700
C	4.38820000	-3.55106200	-0.69208700
C	2.17967200	-4.31902400	0.06033400
C	5.59748800	-2.79775400	-0.54484400
C	4.29179900	-4.42777000	-1.83785700
C	2.10868900	-5.20826600	-1.07870000
C	6.60968200	-2.87651000	-1.46533000
H	5.71679300	-2.16075800	0.32361400
C	5.36676000	-4.47470200	-2.77998400
C	3.15959400	-5.23117900	-1.99861100
C	6.49391400	-3.71902000	-2.60647100
H	7.51523800	-2.29315500	-1.32141700

H	5.26754500	-5.13507300	-3.63831000
H	3.10084400	-5.89952400	-2.85553000
H	7.30502600	-3.76562300	-3.32794500
C	2.28579000	4.09569000	-0.83730600
C	1.17902500	4.69048100	-0.18266500
C	2.35367800	4.07717400	-2.25131400
C	1.05428300	4.74041900	1.24326900
C	0.12856500	5.29745400	-0.96952100
C	1.30258600	4.70023200	-3.02537300
C	-0.02844700	5.32679600	1.84411900
H	1.83093900	4.29752400	1.85554400
C	-0.98165600	5.90501200	-0.30227500
C	0.22234300	5.29280500	-2.36453100
C	-1.06276800	5.91876300	1.06446200
H	-0.10210200	5.33928900	2.92768300
H	-1.75973900	6.36076700	-0.91012500
H	-0.56441700	5.76385700	-2.95033200
H	-1.91042100	6.38394400	1.56014000
C	-0.02313700	-5.11819300	0.75973600
H	-0.85971000	-5.07263200	1.45090400
C	1.06350600	-4.30618000	0.95659200
H	1.08306900	-3.63001200	1.79940600
C	-0.07660300	-6.00854800	-0.35008900
H	-0.94547700	-6.64574400	-0.48793500
C	0.96034300	-6.04565500	-1.24301400
H	0.93140700	-6.71495600	-2.09978300
C	3.46541500	3.45697400	-4.33811700
H	4.28612500	2.96771300	-4.85558600
C	2.44087400	4.09506000	-5.09479900
H	2.49555500	4.09777800	-6.18002100
C	1.39030500	4.69420500	-4.45380600
H	0.59700200	5.17717800	-5.01955700
C	3.42364800	3.44856900	-2.96813600
H	4.20474600	2.94800400	-2.40749800
C	0.99801600	-2.00703500	-3.88849400
H	1.48985600	-2.97628400	-3.74416400
H	1.18532500	-1.69724900	-4.92448500
H	1.49145900	-1.30168200	-3.21690100
C	-1.04191400	-3.28684800	-4.52258700
H	-0.87152500	-3.05567100	-5.58140700
H	-0.51666200	-4.22276900	-4.29958100
H	-2.11080600	-3.45518400	-4.36252900

TS-1-2-2S-2

l imaginary frequencies

H = -5198.717305

G = -5198.909283

E(M06-2X-DCM) = -5199.553965

O	3.47865800	0.29668900	-0.05617900
O	2.07623900	-1.85943900	-0.44965600
P	2.02250600	-0.37703700	0.21547900
O	1.94386100	-0.43454100	1.73761000
N	0.76111900	0.35973200	-0.43785200
S	0.15388500	0.35167200	-1.90927800
C	-0.68554600	-1.32140600	-2.13871700
F	-1.66102900	-1.19140400	-3.04614400
F	0.19082700	-2.22507100	-2.57716600
F	-1.22088400	-1.74723400	-0.98715600
C	-0.25063000	3.35421400	2.94077400
C	-1.01111400	2.26190700	3.79484800
H	-0.54778200	2.28011500	4.78869700
H	-2.03735500	2.61833600	3.90460500
C	-2.21625000	0.17471300	2.84492600
C	-3.50127600	0.59397000	3.25324500
C	-2.12097600	-0.94227900	1.98274600
C	-4.63769500	-0.09477000	2.83790900
H	-3.61944700	1.43825700	3.92073300
C	-3.26071400	-1.59993400	1.53923400
H	-1.14953800	-1.26129300	1.62416700
C	-4.52400600	-1.18384700	1.97389800
H	-5.61834900	0.23755400	3.16358700
H	-3.16233700	-2.42989000	0.84675800
H	-5.42052600	-1.68685400	1.62398500
C	-1.00186500	0.81338400	3.35929200
C	-1.14564000	3.91478300	1.80456800
H	-0.54112600	4.61206000	1.20902100
H	-1.97650000	4.47665800	2.23481200
N	-1.73669900	2.92920300	0.91286500
C	-3.07731100	2.83274300	0.65528000
N	-3.33100500	1.99203900	-0.39970800
C	-4.50089000	1.36642500	-0.85472100
C	-5.72936300	1.35403700	-0.18378300
C	-4.37666800	0.63914600	-2.05488900
C	-6.78704700	0.59624900	-0.69195400
C	-5.44765600	-0.09315900	-2.55151500
H	-3.43227900	0.64066700	-2.58716500
C	-6.66921300	-0.12953500	-1.87308900
H	-7.50189800	-0.70510900	-2.25855300

C	-5.27825300	-0.92440400	-3.79545300
C	-8.03845900	0.50172600	0.13783000
F	-4.21854300	-0.53661700	-4.53393200
F	-6.37318000	-0.86291900	-4.58708300
F	-5.09362300	-2.23282300	-3.49299200
F	-9.07357700	-0.02986900	-0.54494100
F	-8.43212600	1.70154900	0.61011600
F	-7.83642300	-0.29320800	1.22757100
S	-4.24826700	3.67187100	1.54060500
H	-5.84982200	1.92153800	0.72732000
C	0.15551500	0.04288200	3.54836000
H	-2.50485400	1.70107600	-0.92515300
H	0.91665300	0.47052900	4.20004400
H	0.00885900	-1.02768400	3.69093300
O	1.11387000	0.41922400	-3.01511400
H	-1.10538300	2.46896400	0.26133600
O	-0.97306100	1.31236400	-1.91893300
H	0.93299800	-0.09147400	2.45804200
C	5.09119300	-4.56718800	0.62272100
C	5.32384900	-3.59333800	-0.34185800
C	4.30149100	-2.71790400	-0.74257300
C	2.79059900	-3.77230500	0.86346900
C	3.82502900	-4.66257000	1.19737600
C	3.90612500	0.59408300	-1.36310200
C	4.32294600	-0.43640700	-2.20324600
C	4.51645900	-0.16264900	-3.56625500
C	4.45677300	1.14145000	-4.04260800
C	4.21242000	2.17813300	-3.14411800
C	3.91310100	1.93549200	-1.79270900
H	3.62225600	-5.43089900	1.93754500
H	4.22183000	3.20704000	-3.49059800
C	4.76953200	-1.86920800	-1.91895500
C	6.32005400	-1.89562800	-1.67393400
H	6.88879700	-1.68108400	-2.58313000
H	6.57088500	-1.12533600	-0.93536600
H	4.14754500	-1.51310500	-5.23185000
H	5.81716400	-1.50650000	-4.67372100
C	3.06851300	-2.78495800	-0.10008000
H	5.88167300	-5.24875000	0.92624800
H	4.61652300	1.35789000	-5.09564600
C	6.60571000	-3.29017500	-1.08311600
H	6.78946400	-4.03085200	-1.87408100
H	7.48465700	-3.30333400	-0.42878400
C	4.77375000	-1.44085800	-4.33564300

C	4.44428600	-2.53534200	-3.29522700
H	4.99853000	-3.46627800	-3.45154300
H	3.37382500	-2.76792000	-3.32808900
C	3.69918300	3.10692200	-0.88480300
C	4.65180500	3.39143800	0.12797900
C	2.62481100	4.00173400	-1.11989800
C	5.78238000	2.55394100	0.39600700
C	4.51867600	4.59692500	0.91549900
C	2.51824200	5.21440900	-0.33848000
C	6.68546200	2.86096000	1.37991200
H	5.92770800	1.66175600	-0.20151900
C	5.48036900	4.87856400	1.93597100
C	3.46545300	5.47807700	0.65455100
C	6.53242400	4.03551400	2.16934000
H	7.53248400	2.20387600	1.55827300
H	5.35675700	5.78725800	2.52063200
H	3.38285800	6.39321600	1.23804800
H	7.25733300	4.26166100	2.94657700
C	1.45851300	-3.94353900	1.52423000
C	0.36401800	-4.45811500	0.78646700
C	1.32933800	-3.69841100	2.91353600
C	0.44163500	-4.75892200	-0.61112600
C	-0.88734800	-4.72564200	1.45974200
C	0.07832400	-3.99115400	3.57721400
C	-0.63746300	-5.25206600	-1.29666200
H	1.37599000	-4.58813300	-1.13300400
C	-1.98968200	-5.24124100	0.70725100
C	-0.99410300	-4.49140100	2.83339700
C	-1.87420900	-5.49279700	-0.63347100
H	-0.55092600	-5.46391300	-2.35871200
H	-2.92273800	-5.43668300	1.23069700
H	-1.93426300	-4.70663700	3.33688100
H	-2.71848700	-5.88389700	-1.19431900
C	0.58021700	4.63667700	-2.30075100
H	-0.18379800	4.40863700	-3.03811900
C	1.61023800	3.75387400	-2.10105000
H	1.65123500	2.84098300	-2.68271200
C	0.49349900	5.84044400	-1.54487800
H	-0.32495800	6.53219400	-1.72465100
C	1.43732200	6.11722600	-0.59171200
H	1.38279000	7.03157500	-0.00499100
C	2.24052700	-2.95061400	5.05558300
H	3.06285900	-2.53687400	5.63301500
C	1.01376300	-3.26383300	5.70838200

H	0.91481800	-3.09837600	6.77776600
C	-0.03647800	-3.76230900	4.98534700
H	-0.98203300	-3.99676600	5.46856500
C	2.39141200	-3.15623000	3.70874000
H	3.32384300	-2.89223600	3.22431800
C	1.08917800	2.86192000	2.37889700
H	1.62882400	3.70037000	1.92809500
H	1.73191400	2.44302100	3.16045000
H	0.95928000	2.10211700	1.60573600
C	0.01656200	4.53888400	3.89518500
H	0.74413800	4.26324700	4.66713600
H	0.42615600	5.39174200	3.34186700
H	-0.90216300	4.87131700	4.39300200

TS-1-2-2R

1 imaginary frequencies

H = -5198.719019

G = -5198.910972

E(M06-2X-DCM) = -5199.560738

O	1.87423700	-1.85267100	-0.43973300
O	3.27530400	0.27672300	0.11414600
P	1.76889800	-0.28497600	-0.08111300
O	1.10599600	-0.10082600	1.30588800
N	1.12552300	0.47706800	-1.32417300
S	-0.26160300	0.08998300	-2.02180600
C	0.28944900	-0.83379300	-3.55495000
F	-0.78102800	-1.29273700	-4.20523900
F	1.08377200	-1.86467100	-3.23954900
F	0.96679800	-0.00286400	-4.35744800
C	-0.33080200	1.06362400	4.78930500
C	-0.45272300	2.48435300	4.13686800
H	0.26871900	3.13013000	4.65694200
H	-1.44852000	2.84440300	4.39633300
C	-1.26983500	3.20235800	1.78826200
C	-2.37621200	3.90804000	2.31006300
C	-1.19516900	3.04348100	0.38495100
C	-3.35056200	4.43692900	1.46745600
H	-2.47356900	4.07706600	3.37540300
C	-2.18552100	3.54244300	-0.45061900
H	-0.37955500	2.48942800	-0.06416300
C	-3.26793400	4.24617600	0.08723500
H	-4.18716400	4.98155600	1.89519000
H	-2.11206800	3.35555100	-1.51632600
H	-4.05612700	4.61538500	-0.56236000

C	-0.20479800	2.67286100	2.65355100
C	-1.45582600	0.11786600	4.29360700
H	-1.24366600	-0.89606200	4.65485200
H	-2.40719500	0.42661800	4.72992800
N	-1.68233900	0.08131000	2.85259700
C	-2.93312600	0.15554800	2.29318000
N	-2.94348100	-0.11558600	0.95037700
C	-4.04265700	-0.05609900	0.05968300
C	-4.95109000	1.00846000	0.05112800
C	-4.16616700	-1.07034900	-0.89366900
C	-5.97312400	1.03767000	-0.89651200
C	-5.19748800	-1.02967300	-1.83334700
H	-3.44809700	-1.88170400	-0.91040500
C	-6.11272800	0.02029500	-1.84252800
H	-6.91390100	0.04886000	-2.56980300
C	-5.30541600	-2.16050400	-2.81968600
C	-6.87987800	2.23767200	-0.93413100
F	-4.17264500	-2.30751600	-3.54410200
F	-5.51180600	-3.35018800	-2.19427500
F	-6.32236400	-1.99112600	-3.69019100
F	-8.00756500	2.00636800	-1.63990800
F	-7.24654600	2.63561600	0.30245100
F	-6.26750000	3.30539400	-1.51470400
S	-4.31992400	0.54710400	3.17578600
H	-4.85396300	1.80535400	0.77432300
C	1.06156700	2.40286300	2.13274300
H	-2.09131800	-0.45815100	0.50621000
H	1.88205800	2.29527000	2.83861500
H	1.34395200	2.87564600	1.19418400
O	-1.05510300	-0.88377900	-1.23967800
H	-0.93751500	-0.31456900	2.28414900
O	-0.92763700	1.28412100	-2.54458900
H	1.01041100	1.08283900	1.69258900
C	5.39716800	0.61380800	-3.48115500
C	5.27103200	-0.61902800	-2.85113800
C	4.66768600	-0.71905300	-1.58618600
C	4.22550500	1.68496800	-1.62009700
C	4.91532500	1.75603200	-2.84139400
C	2.65173300	-2.79899500	0.23847300
C	4.02690900	-2.82937000	0.00844200
C	4.81399900	-3.73065000	0.74426300
C	4.22580000	-4.66103500	1.59347300
C	2.83882100	-4.68178600	1.71891900
C	2.01628500	-3.74376700	1.06907000

H	5.04015000	2.72984800	-3.30511800
H	2.36566900	-5.42874100	2.34852700
C	4.90238500	-2.11916600	-1.02438000
C	4.97995600	-2.93409200	-2.35890500
H	3.95959700	-3.13292300	-2.70668900
H	5.48711100	-3.89560300	-2.23432700
H	6.67696300	-4.33603200	-0.18248500
H	6.89470000	-3.51406400	1.35858100
C	4.07543500	0.41371100	-1.03678300
H	5.87106200	0.69381600	-4.45608900
H	4.83466100	-5.37436700	2.14307600
C	5.69150100	-1.98528900	-3.34847600
H	5.39171600	-2.15868700	-4.38809000
H	6.78259600	-2.10927100	-3.31097800
C	6.28292500	-3.52791900	0.44935600
C	6.28814300	-2.17749300	-0.29374800
H	6.33715900	-1.35588400	0.43033300
H	7.12869900	-2.06228700	-0.98411200
C	0.53571000	-3.81794300	1.26895400
C	0.00287200	-3.71687200	2.58178200
C	-0.32354100	-4.08967100	0.17304800
C	0.80584400	-3.44918900	3.73963600
C	-1.41696600	-3.89586400	2.79169800
C	-1.74699100	-4.21160200	0.39537500
C	0.26561700	-3.43637200	5.00056300
H	1.86487800	-3.25875800	3.61254500
C	-1.94344600	-3.85766200	4.12125000
C	-2.25282300	-4.11632400	1.69398200
C	-1.12724800	-3.65467600	5.20136500
H	0.90730700	-3.25051600	5.85816700
H	-3.01294200	-4.00088700	4.25296300
H	-3.32251100	-4.22902000	1.85659500
H	-1.53758600	-3.64443000	6.20738200
C	3.72306100	2.94312800	-0.98563200
C	2.72090700	3.71127300	-1.62949500
C	4.32249200	3.40983500	0.21214900
C	2.05479800	3.27938600	-2.82202700
C	2.32410800	4.98233400	-1.06341200
C	3.89747700	4.67087300	0.77757600
C	1.09825400	4.05466400	-3.42268400
H	2.28857500	2.30483400	-3.23120100
C	1.32708300	5.76368600	-1.72769200
C	2.91757000	5.42253700	0.12279400
C	0.73484500	5.31920900	-2.87829600

H	0.59352000	3.68914000	-4.31184900
H	1.04806700	6.71980300	-1.29129000
H	2.61170200	6.37757400	0.54552600
H	-0.02352000	5.92004100	-3.37284500
C	-0.71510700	-4.50603200	-2.20399600
H	-0.32450000	-4.62947000	-3.21018000
C	0.14879100	-4.28201900	-1.16441800
H	1.21421400	-4.24614300	-1.35705100
C	-2.11997200	-4.57022200	-1.98626400
H	-2.79439200	-4.71504900	-2.82444500
C	-2.61609300	-4.44260700	-0.71738200
H	-3.68591400	-4.50203200	-0.53558300
C	5.91889700	3.17969600	2.05147900
H	6.70887400	2.61857400	2.54361400
C	5.47842100	4.41059700	2.61570300
H	5.92964900	4.77483800	3.53465900
C	4.49926000	5.13354300	1.98994400
H	4.16156700	6.08234300	2.40056300
C	5.36439300	2.70062600	0.89319500
H	5.72513200	1.76837000	0.47373800
C	-0.57656200	1.26822500	6.30254600
H	0.23288600	1.85119100	6.75737200
H	-1.52229900	1.78854200	6.49261700
H	-0.61816100	0.30113800	6.81686200
C	1.06108200	0.42015000	4.63597600
H	1.85203300	1.10821800	4.95946400
H	1.11754200	-0.46891100	5.27368700
H	1.28410600	0.09305300	3.61998100

TS-EF-1S-B3LYP-D3 (BJ)

1 imaginary frequencies

H = -5199.192896

G = -5199.374211

E(M06-2X-DCM) = -5199.57817

O	2.29432700	-1.78133500	-0.21143600
O	2.52865500	0.77811500	0.03842100
P	1.41351600	-0.41311700	-0.10944500
O	0.62456500	-0.36681400	1.16715700
C	4.53261400	-2.71865300	3.18971500
C	5.05549700	-1.89731200	2.19554500
C	4.32246900	-1.64836400	1.02782400
C	2.46800800	-2.97251900	1.89802400
C	3.25946300	-3.26696600	3.02090000
C	3.48046500	0.92360000	-0.97347900

C	4. 59349400	0. 08745300	-1. 00536500
C	5. 43867700	0. 12743600	-2. 12593400
C	5. 22918000	1. 04969500	-3. 14499300
C	4. 16953900	1. 94974800	-3. 03785800
C	3. 27132400	1. 89925500	-1. 96147200
H	2. 84213500	-3. 91260200	3. 78734900
H	4. 00666000	2. 69675900	-3. 80836800
C	5. 16386200	-0. 87591600	0. 02883300
C	6. 14632300	-0. 14578900	1. 00205000
H	5. 65046700	0. 75345700	1. 38517000
H	7. 07040000	0. 16476700	0. 50610500
H	7. 47558700	-0. 51324300	-1. 76170400
H	6. 63996900	-1. 48262800	-2. 97223000
C	3. 03497400	-2. 15009700	0. 90895500
H	5. 10082400	-2. 92980900	4. 09170800
H	5. 88349900	1. 07579200	-4. 01204200
C	6. 37029300	-1. 14952700	2. 15525300
H	6. 60581100	-0. 65791500	3. 10545500
H	7. 20547200	-1. 82796300	1. 93363800
C	6. 50092500	-0. 94461100	-2. 02845200
C	5. 96012900	-1. 84637800	-0. 90040000
H	5. 25914800	-2. 57903200	-1. 31503300
H	6. 74007400	-2. 39144000	-0. 36089700
C	2. 17447300	2. 90643100	-1. 88362100
C	1. 15276500	2. 91310900	-2. 85742400
C	2. 22888300	3. 92319000	-0. 90133700
C	1. 00655700	1. 86297200	-3. 81638700
C	0. 18965300	3. 98834600	-2. 87559800
C	1. 24177600	4. 97812900	-0. 91364800
C	-0. 01131100	1. 87717600	-4. 73029200
H	1. 68251100	1. 02079700	-3. 77291100
C	-0. 83428500	3. 98527200	-3. 87144100
C	0. 25691100	4. 98792500	-1. 90444400
C	-0. 93571900	2. 95964800	-4. 77130200
H	-0. 13210600	1. 03977800	-5. 40915500
H	-1. 54800200	4. 80487900	-3. 87652600
H	-0. 48120800	5. 78651200	-1. 91194600
H	-1. 73173700	2. 95641200	-5. 51055700
C	1. 07155200	-3. 47890500	1. 79006700
C	0. 11691700	-3. 10218700	2. 76640200
C	0. 69417500	-4. 30242500	0. 70568900
C	0. 41244100	-2. 21223400	3. 84768400
C	-1. 23668000	-3. 59334600	2. 66211600
C	-0. 67377900	-4. 74771300	0. 58992000

C	-0.54135900	-1.86622200	4.76917400
H	1.40884400	-1.79388100	3.92033600
C	-2.20382700	-3.19858100	3.63684800
C	-1.59301500	-4.40662900	1.58251000
C	-1.87126700	-2.36125400	4.66687800
H	-0.28638800	-1.19393800	5.58397700
H	-3.21913100	-3.57177900	3.53022800
H	-2.62209600	-4.74295900	1.48904500
H	-2.61692900	-2.06051300	5.39657700
C	3.29759600	4.99952700	1.01504600
H	4.09532500	5.02647900	1.75235500
C	3.25296900	3.98304800	0.09608700
H	4.01372000	3.21131000	0.10837100
C	2.31585400	6.03110700	1.00565300
H	2.36943300	6.83300500	1.73700600
C	1.31638300	6.01244300	0.06941600
H	0.56383000	6.79681900	0.04502500
C	1.19162200	-5.43462800	-1.39452200
H	1.90434000	-5.70958400	-2.16665000
C	-0.17103000	-5.82166600	-1.53097100
H	-0.48727800	-6.37307900	-2.41146400
C	-1.07315600	-5.50072900	-0.55589800
H	-2.11851900	-5.77786400	-0.64782600
C	1.61042600	-4.70955100	-0.31218800
H	2.65157900	-4.42279600	-0.22691100
C	0.77548200	2.76688800	3.72558800
C	0.26919100	3.50448000	2.44347100
H	0.69656900	4.51623600	2.44732200
H	0.71740800	3.03434900	1.56892100
C	-1.74062400	3.44009000	0.86044600
C	-1.17676900	2.45745800	0.01881900
C	-2.89485700	4.11919000	0.40891400
C	-1.76977300	2.13134400	-1.19266300
H	-0.30792200	1.89705700	0.33472200
C	-3.47516700	3.80439700	-0.81356000
H	-3.31840900	4.91937900	1.00647200
C	-2.92297000	2.79716900	-1.60798800
H	-1.34124300	1.35464400	-1.81132800
H	-4.36843900	4.32808200	-1.13827800
H	-3.38709700	2.52539800	-2.54877700
C	-1.20490800	3.68638200	2.19906300
C	-0.21444000	1.67044200	4.19032400
H	-1.04921000	2.08179000	4.75386200
H	0.31492900	0.97776800	4.85651700

N	-0.72727200	0.92664700	3.05903700
C	-1.98552300	0.60449700	2.75854400
N	-2.12571700	-0.24580600	1.72155200
C	-3.24506100	-0.47421900	0.88699800
C	-4.17929400	0.51982300	0.57896800
C	-3.31972700	-1.71903800	0.26512800
C	-5.19467000	0.24037300	-0.32917200
C	-4.33378500	-1.97577400	-0.65641700
H	-2.56801500	-2.46758300	0.47150600
C	-5.28455800	-1.00614200	-0.95433100
H	-6.07781100	-1.21149600	-1.66214300
C	-4.36469500	-3.32234600	-1.32777600
C	-6.17416200	1.31327000	-0.71257300
F	-3.31329300	-3.51102400	-2.14251300
F	-5.48656300	-3.49757500	-2.05983100
F	-4.33117700	-4.32782900	-0.40879100
F	-7.43432000	0.83204900	-0.79401700
F	-5.88806500	1.84383400	-1.92972000
F	-6.18612400	2.33923900	0.16633600
S	-3.33013600	1.25439900	3.64458200
H	-4.10500800	1.50119800	1.02151600
H	-1.24544400	-0.64883900	1.37723400
H	-0.01977300	0.51358500	2.43349500
C	-2.08682900	4.01587900	3.22875300
H	-1.68676900	4.36740200	4.17525200
H	-2.62247300	2.76941600	3.51606300
H	-3.05961600	4.42933600	2.96749500
N	0.70392800	-0.20090500	-1.53048700
S	-0.34134700	-1.26256900	-2.11045100
O	-1.37636300	-0.59132600	-2.90496600
O	-0.75244100	-2.28152200	-1.13041600
C	0.66855100	-2.18602400	-3.38194900
F	0.97446000	-1.37045200	-4.40680400
F	-0.04113000	-3.21620900	-3.85207000
F	1.80843700	-2.64525300	-2.85771800
C	2.12430100	2.11342200	3.35774700
H	2.81877400	2.86757500	2.97427100
H	2.57687800	1.64402500	4.23919900
H	2.01550800	1.35298900	2.57880300
C	1.00887600	3.73399100	4.89816300
H	1.36463500	3.19012800	5.78119000
H	1.77121300	4.47490600	4.63456000
H	0.10143200	4.27371300	5.18657200

TS-EF-1S-1-B3LYP-D3 (BJ)

1 imaginary frequencies

H = -5199.184356

G = -5199.36683

E(M06-2X-DCM) = -5199.57346

O	1.93475300	-2.28511200	-0.38049800
O	2.82376300	0.12230100	-0.05793400
P	1.44727900	-0.72364600	-0.35076600
O	0.53939800	-0.44839700	0.81251900
C	4.14837000	-3.76576900	2.84501800
C	4.77732500	-3.12522900	1.78235400
C	4.03501800	-2.66764900	0.68472800
C	1.98620400	-3.44857700	1.74901700
C	2.76406000	-3.93706500	2.81075400
C	3.77360500	0.15433400	-1.08232600
C	4.59178700	-0.94715100	-1.29592400
C	5.33809100	-1.02140200	-2.48128200
C	5.35549500	0.04587000	-3.37311500
C	4.64970000	1.20905500	-3.05528600
C	3.84371100	1.28558300	-1.91115300
H	2.25757900	-4.44225600	3.62748700
H	4.70168100	2.07492300	-3.70818900
C	4.95585500	-2.11161300	-0.38773000
C	6.19918100	-1.72934500	0.48549700
H	6.02126400	-0.74141100	0.92548600
H	7.11865400	-1.67369400	-0.10390700
H	7.11272100	-2.26566500	-2.41114000
H	5.90556400	-2.82641700	-3.56391600
C	2.65219800	-2.80282700	0.69302200
H	4.72260300	-4.12664800	3.69405400
H	5.92667700	-0.01031600	-4.29566500
C	6.24086900	-2.79244300	1.60168900
H	6.70984800	-2.42632500	2.52139000
H	6.80887900	-3.67816000	1.28509600
C	6.03159700	-2.36414900	-2.57903800
C	5.35982200	-3.17999200	-1.44970100
H	4.44872000	-3.65759100	-1.82577700
H	6.00459400	-3.95899500	-1.03180100
C	3.19349400	2.57531900	-1.53222800
C	2.10803200	3.09685300	-2.26826800
C	3.76299200	3.32455700	-0.47424500
C	1.49834000	2.37835800	-3.34209600
C	1.58357200	4.40434400	-1.93949800
C	3.20908700	4.61432200	-0.13421400

C	0.47072300	2.92662700	-4.06299100
H	1.83529000	1.37355900	-3.55781100
C	0.51667500	4.94126400	-2.72149000
C	2.13673600	5.11834400	-0.87449900
C	-0.01644600	4.22937600	-3.76076800
H	0.00477000	2.34118100	-4.84751300
H	0.13207400	5.92446800	-2.46283200
H	1.73357100	6.09832900	-0.62698800
H	-0.83359300	4.64446900	-4.34387600
C	0.50664800	-3.62757600	1.76090200
C	-0.27539800	-2.95763200	2.72930800
C	-0.10316000	-4.48550700	0.81981700
C	0.28604600	-2.06931400	3.70017100
C	-1.70580100	-3.15214700	2.74669100
C	-1.53623400	-4.66179700	0.83921400
C	-0.50195500	-1.44741000	4.63258400
H	1.35466100	-1.89102400	3.68508600
C	-2.49421000	-2.45740500	3.71456700
C	-2.29702800	-3.99885500	1.80469100
C	-1.91330700	-1.63262200	4.63899700
H	-0.04955900	-0.79443100	5.37371900
H	-3.57149400	-2.60017200	3.69703900
H	-3.37694000	-4.12209600	1.80381900
H	-2.52255900	-1.10801300	5.36815600
C	5.43748300	3.62528600	1.28076400
H	6.30488600	3.26042400	1.82327800
C	4.90416600	2.87645000	0.26447800
H	5.35251600	1.92516300	0.00355100
C	4.86411900	4.87882100	1.63722900
H	5.29593700	5.45793500	2.44857500
C	3.78274800	5.35572400	0.94492600
H	3.34931700	6.32249900	1.19100400
C	0.01442100	-5.97266700	-1.10779700
H	0.60094900	-6.48604100	-1.86429500
C	-1.40176400	-6.12016600	-1.10167000
H	-1.88072100	-6.73524400	-1.85790700
C	-2.15297900	-5.48861700	-0.14933900
H	-3.23469900	-5.57821400	-0.14072900
C	0.64164500	-5.18886500	-0.17717200
H	1.72011600	-5.08579300	-0.19479800
C	1.09004000	2.91932800	3.19960400
C	0.54230600	3.68851900	1.95619700
H	1.09938400	4.63389000	1.88061900
H	0.82337000	3.14677600	1.05251800

C	-1.59233800	3.98910100	0.57159600
C	-1.28734000	2.98916100	-0.37642600
C	-2.65319900	4.88082200	0.28514500
C	-2.03572500	2.87134500	-1.54322200
H	-0.51663900	2.25270100	-0.18354300
C	-3.38652600	4.76656600	-0.88714300
H	-2.87508300	5.68978000	0.97267600
C	-3.08344000	3.75378100	-1.80057400
H	-1.81383100	2.06519000	-2.22699900
H	-4.19704000	5.46043500	-1.08709600
H	-3.67369100	3.64260400	-2.70378900
C	-0.91203300	4.05932300	1.86493900
C	0.06159200	1.89315400	3.73255700
H	-0.70750600	2.35084500	4.35084500
H	0.58853700	1.16551400	4.36050200
N	-0.57157600	1.18714600	2.63804600
C	-1.87121800	0.98615700	2.40923200
N	-2.14770200	0.17662900	1.37070300
C	-3.36752900	-0.00133700	0.68161200
C	-4.22537500	1.06015500	0.38405700
C	-3.62681300	-1.27254000	0.17768800
C	-5.35651800	0.82355100	-0.39026200
C	-4.76481300	-1.49389500	-0.59505500
H	-2.92649400	-2.07581100	0.36656900
C	-5.64331100	-0.45342400	-0.88024900
H	-6.52736700	-0.62726200	-1.48086900
C	-5.01310900	-2.88780000	-1.09903900
C	-6.23729000	1.97344800	-0.78995800
F	-3.96050900	-3.36233400	-1.79509900
F	-6.10004200	-2.96312300	-1.89279100
F	-5.21302000	-3.75624800	-0.06790000
F	-6.09146700	3.04043800	0.02570700
F	-7.54419800	1.62982300	-0.78324700
F	-5.95787900	2.40101600	-2.04749800
S	-3.10505900	1.72903700	3.38047300
H	-4.00304300	2.05836900	0.73066800
H	-1.33396200	-0.27125500	0.92886000
H	0.06025000	0.66853700	2.01033400
C	-1.66897200	4.39444600	2.99125200
H	-1.15893700	4.63675900	3.91816800
H	-2.27135500	3.21469100	3.23714400
H	-2.60687900	4.92661200	2.84028700
N	1.03550400	-0.43164000	-1.86769400
S	-0.42035900	-0.55274000	-2.48280700

O	-0.42153000	-0.09571600	-3.87407300
O	-1.49087300	-0.06705400	-1.58701500
C	-0.76589700	-2.38426000	-2.57059000
F	0.29102400	-3.06124300	-3.02410500
F	-1.81040700	-2.61346200	-3.36993300
F	-1.06116300	-2.81791600	-1.33501600
C	2.35290500	2.16759700	2.73726100
H	3.09538800	2.86668500	2.34939800
H	2.80460500	1.63111900	3.58026500
H	2.14355200	1.44214600	1.94661700
C	1.49517700	3.86293900	4.34444300
H	1.88317900	3.28726700	5.19288900
H	2.29060000	4.53749600	4.01000600
H	0.66578600	4.47370300	4.71377200

TS-EF-1S-2-B3LYP-D3 (BJ)

1 imaginary frequencies

H = -5199.184665

G = -5199.366202

E(M06-2X-DCM) = -5199.571799

O	0.92538100	2.66560100	-0.02944100
O	2.51485500	0.63588500	-0.27854700
P	1.06351500	1.08217500	0.35414100
O	0.05641600	0.25881400	-0.39941600
C	1.38740300	3.88367100	-4.00888300
C	2.48905400	3.72440300	-3.17530500
C	2.31819700	3.35947000	-1.83263800
C	-0.09311800	3.21079500	-2.17640500
C	0.11233400	3.64966800	-3.49657600
C	3.66468700	1.16601500	0.31158600
C	4.03023800	2.47873500	0.04222500
C	5.01079900	3.09057400	0.83643100
C	5.69632700	2.35844600	1.80025400
C	5.42367000	0.99581400	1.93807500
C	4.40465400	0.37326200	1.20231400
H	-0.75785300	3.78475600	-4.13088700
H	5.99194300	0.39349200	2.64005400
C	3.64925000	3.40533400	-1.10124900
C	4.63174300	3.18575100	-2.30119200
H	4.70087600	2.10941200	-2.49755500
H	5.63879500	3.55302700	-2.08552900
H	6.08511900	4.74126500	-0.07066200
H	5.15138100	5.20477400	1.34831400
C	1.04368800	3.07348200	-1.35492600

H	1. 51281500	4. 18794700	-5. 04452700
H	6. 45177100	2. 82951600	2. 42302500
C	3. 95689600	3. 88718900	-3. 49631200
H	4. 23117900	3. 44577400	-4. 46062300
H	4. 23409100	4. 94931700	-3. 54216800
C	5. 14651800	4. 55300300	0. 46813900
C	3. 91895300	4. 79265500	-0. 44112200
H	3. 04958100	5. 06148000	0. 16840900
H	4. 07218600	5. 58341400	-1. 18155600
C	4. 22280500	-1. 10559200	1. 29289400
C	3. 72586400	-1. 70672800	2. 46790700
C	4. 67985900	-1. 91012000	0. 22104400
C	3. 20938600	-0. 93786400	3. 55577000
C	3. 71881500	-3. 14668000	2. 58751300
C	4. 62314000	-3. 34928500	0. 33506500
C	2. 74437800	-1. 54638900	4. 69137700
H	3. 14847200	0. 13747700	3. 45567200
C	3. 25976200	-3. 73852600	3. 80294700
C	4. 15100900	-3. 92797600	1. 51568300
C	2. 78954700	-2. 96286300	4. 82745500
H	2. 31397100	-0. 93783300	5. 47845500
H	3. 27526900	-4. 82209500	3. 88363000
H	4. 12210200	-5. 01135700	1. 60215100
H	2. 43110800	-3. 42439000	5. 74347200
C	-1. 47685300	2. 91216300	-1. 70975700
C	-2. 25046500	1. 93380000	-2. 38450000
C	-2. 03916200	3. 64257800	-0. 63825800
C	-1. 76480500	1. 18093800	-3. 50079400
C	-3. 60123400	1. 66586400	-1. 94530700
C	-3. 37450700	3. 33235400	-0. 18352300
C	-2. 56211800	0. 28211000	-4. 16058800
H	-0. 74298100	1. 33241100	-3. 82775700
C	-4. 39510500	0. 71064700	-2. 65058100
C	-4. 11277100	2. 34615900	-0. 83800100
C	-3. 89664900	0. 03989800	-3. 73475700
H	-2. 16814000	-0. 26795700	-5. 01065700
H	-5. 40534200	0. 52075600	-2. 30095200
H	-5. 11522000	2. 11186500	-0. 48851800
H	-4. 51017700	-0. 68194100	-4. 26560400
C	5. 68666900	-2. 16741800	-1. 99255800
H	6. 11630600	-1. 72184900	-2. 88558100
C	5. 24016600	-1. 36211300	-0. 97607000
H	5. 31987300	-0. 28514000	-1. 06764900
C	5. 60345200	-3. 58509900	-1. 88625000

H	5.96099400	-4.20923800	-2.70039600
C	5.08483300	-4.15313500	-0.75230300
H	5.02572400	-5.23405200	-0.65070100
C	-1.90608800	5.37389700	1.07339500
H	-1.35240200	6.17010700	1.56224200
C	-3.20557000	5.03464000	1.54527400
H	-3.62557100	5.56729900	2.39338000
C	-3.91885400	4.04498600	0.92825300
H	-4.90968000	3.77063100	1.27745600
C	-1.34419200	4.70352700	0.02089600
H	-0.35487800	4.97701500	-0.32466100
C	1.75987900	-1.96164500	-3.43171200
C	2.04338800	-2.70344600	-2.09540100
H	3.05921700	-3.12030000	-2.14327400
H	2.09435000	-1.97485400	-1.28416600
C	0.96513200	-4.04667800	-0.22147600
C	0.72041500	-2.96157200	0.64350000
C	0.94605900	-5.35368500	0.30820800
C	0.41923500	-3.18343300	1.98267400
H	0.70042800	-1.94679600	0.26480500
C	0.68469600	-5.56751300	1.65579600
H	1.18080700	-6.19523400	-0.33591300
C	0.40403800	-4.48303100	2.48974800
H	0.19592300	-2.33570500	2.61863900
H	0.69520800	-6.57811700	2.05390700
H	0.18711700	-4.64616500	3.54062500
C	1.16809300	-3.84500900	-1.65804000
C	0.23899200	-1.81320700	-3.65833200
H	-0.20696400	-2.70840700	-4.08433500
H	0.06148800	-0.99826100	-4.37167400
N	-0.44159900	-1.49422900	-2.41645600
C	-1.59772000	-1.97967400	-1.94969800
N	-2.09657200	-1.31328600	-0.89250100
C	-3.33474500	-1.36192200	-0.23291900
C	-3.37301800	-0.73201000	1.01726100
C	-4.50941100	-1.85600600	-0.80275600
C	-4.58913800	-0.57191900	1.67303300
C	-5.71506900	-1.69394500	-0.12252900
H	-4.50172300	-2.31940100	-1.77810900
C	-5.77310200	-1.04672700	1.11035900
H	-6.71864900	-0.91461200	1.62010500
C	-6.98302100	-2.09739900	-0.81868900
C	-4.61510400	0.20564300	2.96240500
F	-7.39023700	-1.12707700	-1.68178900

F	-7.99867400	-2.30474400	0.04324900
F	-6.82618200	-3.22093900	-1.55004600
F	-3.60149100	-0.13305200	3.77636000
F	-5.77106000	0.01749400	3.63929300
F	-4.50904000	1.53664600	2.72470600
S	-2.28791600	-3.43172800	-2.60149900
H	-2.45561600	-0.36636000	1.46692400
H	-1.47334200	-0.57670600	-0.53521900
H	-0.07692500	-0.68652400	-1.89639200
C	0.50926000	-4.70341100	-2.53602900
H	0.80093500	-4.73706200	-3.58125000
H	-0.75842100	-4.10959200	-2.60366500
H	0.12745400	-5.64147900	-2.13474500
N	1.21759100	1.08469700	1.93609000
S	0.14995500	0.77757100	3.06871400
O	0.77102200	0.90617200	4.38718800
O	-0.69441900	-0.40347400	2.79339700
C	-1.06291100	2.18569100	2.96117300
F	-0.43212300	3.36127500	2.95175800
F	-1.91291700	2.15040500	3.98781200
F	-1.75851000	2.05272200	1.81726000
C	2.38877200	-0.55629500	-3.32896400
H	3.45397100	-0.63189800	-3.09165800
H	2.28253500	-0.02039500	-4.27953100
H	1.93220400	0.04669400	-2.54098700
C	2.38587800	-2.67227700	-4.64322500
H	2.15944400	-2.12808200	-5.56779800
H	3.47502700	-2.70806400	-4.53490400
H	2.02975000	-3.69894300	-4.76820500

TS-EF-1R-B3LYP-D3 (BJ)

1 imaginary frequencies

H = -5199.185456

G = -5199.367502

E(M06-2X-DCM) = -5199.571972

O	-3.18844700	0.46088500	-0.98872000
O	-2.12130100	-1.52070000	0.27739400
P	-1.73816000	-0.18579800	-0.60416400
O	-0.93942600	0.66056300	0.34287700
C	-5.68853100	1.51699100	2.18685400
C	-5.68540000	0.21760500	1.68920200
C	-4.89843000	-0.11705200	0.57819600
C	-4.04428900	2.16782900	0.49708500
C	-4.89556800	2.48482500	1.56827100

C	-2.81091400	-2.55644200	-0.34890100
C	-4.18231500	-2.45508500	-0.52790700
C	-4.83238500	-3.39207700	-1.34422100
C	-4.13195400	-4.46911100	-1.87891400
C	-2.77871900	-4.62724300	-1.56508100
C	-2.09308100	-3.67576800	-0.79836700
H	-4.91324800	3.50960300	1.92576500
H	-2.23202100	-5.49350000	-1.92490400
C	-5.20080900	-1.53587100	0.12473100
C	-5.70603200	-2.15358100	1.47094400
H	-4.83285400	-2.45764900	2.05992000
H	-6.33012000	-3.03787200	1.31395900
H	-6.93738500	-3.69385200	-0.92541200
H	-6.62646600	-3.07683100	-2.54515100
C	-4.04859800	0.83881700	0.03597200
H	-6.30729000	1.78282900	3.03974100
H	-4.63145800	-5.19422700	-2.51552300
C	-6.43760400	-0.99725200	2.18459100
H	-6.41705300	-1.09055000	3.27584600
H	-7.49483600	-0.95375500	1.88906700
C	-6.29127600	-3.01956700	-1.50404600
C	-6.33930100	-1.57925900	-0.94331200
H	-6.09726400	-0.86370600	-1.73664100
H	-7.31283600	-1.30555800	-0.52581700
C	-0.68458100	-3.88665700	-0.35626700
C	0.39401200	-3.81015000	-1.26197300
C	-0.45567300	-4.20932000	1.00273300
C	0.21212100	-3.49802700	-2.64424400
C	1.74031200	-4.04220700	-0.78725700
C	0.89566600	-4.40087000	1.47228700
C	1.27747800	-3.45158300	-3.50363900
H	-0.78166900	-3.25477200	-2.99784400
C	2.82134700	-3.99252700	-1.71987200
C	1.95717100	-4.30323100	0.56786900
C	2.59782900	-3.71313400	-3.04193500
H	1.11693600	-3.17012200	-4.53792100
H	3.83122700	-4.15735300	-1.35382300
H	2.97316700	-4.45097600	0.92543000
H	3.43290100	-3.65109800	-3.73236200
C	-3.19433800	3.21416800	-0.13801000
C	-2.22413600	3.90350200	0.62668400
C	-3.39338500	3.54713100	-1.49917100
C	-1.98477500	3.63126100	2.01019500
C	-1.42548000	4.93420800	0.00501500

C	-2.57622400	4.56780900	-2.11092200
C	-1.06150300	4.34420100	2.72979500
H	-2.54963400	2.84106900	2.48878600
C	-0.45849500	5.63859400	0.78665300
C	-1.61523300	5.23027000	-1.34554400
C	-0.28468200	5.36411400	2.11483800
H	-0.90625500	4.11858500	3.78103000
H	0.13662800	6.40433000	0.29564200
H	-1.00420500	6.00023800	-1.81127700
H	0.45562500	5.90403700	2.69756300
C	-1.26578300	-4.71019600	3.25455900
H	-2.09278600	-4.85276700	3.94494500
C	-1.51904000	-4.38717800	1.94581500
H	-2.54215500	-4.27911100	1.60502400
C	0.07091500	-4.86498200	3.71881400
H	0.25462000	-5.11163000	4.76066800
C	1.11738500	-4.71142700	2.84932500
H	2.14290400	-4.82746200	3.18750800
C	-4.55534700	3.26672500	-3.62684200
H	-5.32261100	2.77708200	-4.21955400
C	-3.72585400	4.25136800	-4.23245900
H	-3.86058700	4.49743900	-5.28166400
C	-2.76899400	4.88598200	-3.48974300
H	-2.13359700	5.64774600	-3.93426100
C	-4.39690200	2.93023900	-2.30927500
H	-5.04549900	2.18542200	-1.86485300
N	-1.19340700	-0.64580600	-2.03605500
S	0.04701100	-0.03615400	-2.80599400
O	0.16019300	-0.61712500	-4.14120100
O	1.27811900	0.05821300	-1.98124500
C	-0.37366800	1.75981400	-3.10284700
F	-1.58254800	1.86818300	-3.65465100
F	0.53369200	2.31349900	-3.91247200
F	-0.36995500	2.43011000	-1.93590800
C	-0.79352300	-0.29643400	3.95434600
C	-0.16559900	1.13054900	3.85234000
H	-0.53246900	1.70961500	4.71410800
H	-0.58565500	1.62029700	2.97710100
C	1.92833300	2.21185000	2.83448300
C	1.35904700	2.35873100	1.55191900
C	3.14393300	2.88185000	3.10375700
C	2.01401200	3.07997600	0.56041400
H	0.43448100	1.86590100	1.28886200
C	3.77744600	3.63180200	2.12086600

H	3.58074300	2.83421000	4.09551900
C	3.22633800	3.71250800	0.83799500
H	1.57075700	3.12532800	-0.42830300
H	4.71760000	4.12570800	2.34100700
H	3.74821200	4.26234800	0.06099100
C	1.32809200	1.31929100	3.83129200
C	0.02022000	-1.35484700	3.16154200
H	0.76443200	-1.83451100	3.79363100
H	-0.66441800	-2.13347500	2.81810300
N	0.70663600	-0.81510300	1.99963900
C	1.99151800	-0.97226700	1.68023300
N	2.34787600	-0.62207400	0.43256500
C	3.66093200	-0.36612400	-0.03407500
C	4.52736900	0.48091400	0.65828300
C	4.03926900	-0.90656000	-1.25904000
C	5.78631600	0.75232900	0.13113400
C	5.31254300	-0.64421000	-1.76382300
H	3.34301100	-1.52414700	-1.80839300
C	6.19699900	0.18234600	-1.07675000
H	7.18366000	0.38471100	-1.47385800
C	5.71538800	-1.32873400	-3.04030400
C	6.67126300	1.74538300	0.82865800
F	4.79018500	-1.16903600	-4.00807900
F	6.89373900	-0.87602800	-3.51646900
F	5.84831700	-2.66870500	-2.85275500
F	7.98009600	1.50754400	0.60265100
F	6.42653800	3.01383700	0.40589800
F	6.47999900	1.74494700	2.16750300
S	3.16143500	-1.55518600	2.82761700
H	4.21560600	0.93245700	1.58848900
H	1.62490600	-0.45703500	-0.28133400
H	0.10179700	-0.34225900	1.30528900
C	2.15972500	0.61413300	4.70540500
H	1.71511500	0.13386500	5.57188700
H	2.54436100	-0.42282900	3.93779600
H	3.17259900	0.98093400	4.86447400
C	-2.21943600	-0.17981500	3.37649900
H	-2.80814400	0.55375200	3.94007200
H	-2.73649100	-1.14376600	3.43593200
H	-2.20207200	0.12930400	2.33141800
C	-0.91601700	-0.80464800	5.40211400
H	-1.39277900	-1.79177200	5.40895400
H	-1.53768300	-0.12956300	6.00080500
H	0.05148700	-0.91130000	5.90092800

TS-EF-1R-1-B3LYP-D3 (BJ)

1 imaginary frequencies

H = -5199.185576

G = -5199.367288

E(M06-2X-DCM) = -5199.569618

O	-2.93907500	0.87467000	0.06243000
O	-2.16034100	-1.56047000	-0.00574600
P	-1.59190600	-0.04027300	-0.09819500
O	-0.63523500	0.15583900	1.02632100
C	-5.17203200	0.38936000	3.56551800
C	-5.42745300	-0.39144300	2.44306600
C	-4.70571600	-0.19310500	1.25768800
C	-3.36145800	1.51241900	2.36555000
C	-4.15204000	1.33932500	3.51336500
C	-3.02264800	-2.00447700	-1.00835700
C	-4.37367600	-1.67653100	-0.95758300
C	-5.18111200	-1.95475100	-2.07143600
C	-4.67386500	-2.66117700	-3.15653300
C	-3.34252300	-3.07575000	-3.13561300
C	-2.48118000	-2.73339200	-2.08038500
H	-3.92103400	1.93656100	4.38998800
H	-2.93623500	-3.64032600	-3.96855200
C	-5.23591500	-1.09722000	0.15765200
C	-5.85582100	-2.24635000	1.02144000
H	-5.05490800	-2.93893200	1.30295300
H	-6.61462100	-2.81420200	0.47596400
H	-7.30426400	-2.13484600	-1.66064400
H	-6.91030700	-0.83677000	-2.78369000
C	-3.67882300	0.74196300	1.23352800
H	-5.73807400	0.24624300	4.48194300
H	-5.30175000	-2.88596900	-4.01448500
C	-6.39717900	-1.53974200	2.28126600
H	-6.42492200	-2.19519800	3.15823700
H	-7.42151200	-1.17501000	2.12289500
C	-6.56000500	-1.35919300	-1.88691800
C	-6.35542100	-0.41140900	-0.68485700
H	-5.98219300	0.55779300	-1.03387500
H	-7.26614500	-0.23658700	-0.10441200
C	-1.04690900	-3.13049900	-2.14235300
C	-0.27183700	-2.72803600	-3.25736200
C	-0.47406900	-3.94976500	-1.13927200
C	-0.72709900	-1.75658400	-4.20404100
C	1.05381900	-3.27125600	-3.43879800

C	0.89089200	-4.40091700	-1.28415500
C	0.04259800	-1.39612300	-5.27741000
H	-1.67220200	-1.26048600	-4.02784600
C	1.80320300	-2.90750200	-4.60024900
C	1.59601100	-4.09541300	-2.45001200
C	1.31329400	-1.99762300	-5.49682000
H	-0.30928900	-0.62357500	-5.95389200
H	2.78793600	-3.34776300	-4.73595100
H	2.59716300	-4.50059000	-2.58173700
H	1.90238900	-1.71033100	-6.36315500
C	-2.18098600	2.42040900	2.40911500
C	-1.12234800	2.11672900	3.29910500
C	-2.10573700	3.55554800	1.57335600
C	-1.09120700	0.92604000	4.09245300
C	0.01625200	2.99913300	3.37712800
C	-0.96904700	4.44020100	1.67407200
C	-0.02877000	0.63866800	4.90909800
H	-1.90779600	0.22029500	4.00839300
C	1.10468600	2.66598100	4.24158800
C	0.04807300	4.14922600	2.58532800
C	1.08736000	1.51882300	4.98689800
H	-0.01359100	-0.29332900	5.46553400
H	1.95911600	3.33665700	4.27461500
H	0.89497500	4.82563700	2.67502500
H	1.92854000	1.26663200	5.62572000
C	-0.57369800	-5.10400000	1.01021400
H	-1.12724100	-5.37979400	1.90215400
C	-1.18392300	-4.36822200	0.02988400
H	-2.22191800	-4.08344500	0.14412400
C	0.78716100	-5.50096100	0.88315000
H	1.25551800	-6.06799000	1.68123500
C	1.49313800	-5.16692100	-0.23928500
H	2.53474900	-5.45546900	-0.35125300
C	-3.00687800	4.97335700	-0.19560800
H	-3.77954500	5.18126900	-0.92966200
C	-1.88770100	5.84564800	-0.08990600
H	-1.82126400	6.71606700	-0.73649900
C	-0.90850200	5.59169800	0.83084200
H	-0.06104200	6.26476500	0.93839000
C	-3.12001100	3.88044000	0.62070600
H	-3.98505600	3.23433800	0.53921100
N	-1.12619100	0.17043700	-1.63528900
S	-0.62494200	1.55572700	-2.18188600
O	0.34349500	1.40105400	-3.27653300

O	-0.27101900	2.54499800	-1.12272900
C	-2.10112900	2.31235500	-3.03762900
F	-2.45330500	1.53579700	-4.07131100
F	-1.76701000	3.52469500	-3.49845100
F	-3.14702600	2.43471900	-2.21874900
C	2.92591600	4.75582500	-1.21775200
C	3.60260700	3.67790800	-2.12891100
H	4.17779400	4.22067000	-2.89432800
H	2.82093800	3.15398600	-2.67819600
C	4.37652500	1.25394700	-1.84546200
C	3.09200100	0.74183400	-2.11949200
C	5.45920200	0.34588400	-1.78804300
C	2.88107400	-0.61990700	-2.27917500
H	2.23465600	1.39359000	-2.17417900
C	5.25103400	-1.01362300	-1.97752200
H	6.46817200	0.71122200	-1.62974900
C	3.95977400	-1.50123200	-2.20478500
H	1.87517500	-0.98032100	-2.45560400
H	6.08850300	-1.70061900	-1.92372200
H	3.79329400	-2.56576000	-2.30698300
C	4.55255300	2.66900700	-1.53995000
C	2.63229900	4.24363600	0.21717100
H	3.51118500	4.33686900	0.85326600
H	1.85294300	4.88117300	0.64426300
N	2.17905700	2.86282400	0.29254800
C	2.68004400	1.89721100	1.07945100
N	1.94322800	0.78282900	1.19357000
C	2.34952000	-0.49439700	1.65493600
C	3.51932900	-1.11008000	1.20423200
C	1.46658000	-1.19118700	2.48007400
C	3.79518700	-2.41947400	1.59580400
C	1.76129500	-2.49612500	2.86573600
H	0.54699500	-0.71968400	2.79161300
C	2.92485200	-3.12204100	2.43097100
H	3.14652400	-4.13960400	2.72403200
C	0.81124100	-3.18733100	3.80227100
C	4.99224500	-3.12863500	1.03312000
F	0.92980500	-2.70781100	5.06881200
F	-0.47484900	-3.00400900	3.44192300
F	1.03260500	-4.52003500	3.87096800
F	6.01145000	-2.28292600	0.76294700
F	5.46213100	-4.07663700	1.87133500
F	4.69768800	-3.76361900	-0.13634500
S	4.19077500	2.06524400	1.92112800

H	4.19271700	-0.58339900	0.54336800
H	0.92952300	0.81096500	0.97127500
H	1.28463100	2.66157600	-0.17685900
C	5.53693000	3.05095200	-0.62239600
H	5.78427600	4.10430000	-0.53064600
H	4.93001400	2.73278700	0.51790800
H	6.37789200	2.37865200	-0.45853300
C	1.61174200	5.15646200	-1.91828500
H	1.81271200	5.48131800	-2.94575700
H	1.13510500	5.98850500	-1.38943200
H	0.89522900	4.33271100	-1.95136600
C	3.78899600	6.02347800	-1.07499600
H	3.27307500	6.76403000	-0.45271500
H	3.96472700	6.48127300	-2.05444200
H	4.76073100	5.82931200	-0.61138000

TS-EF-1R-2-B3LYP-D3 (BJ)

1 imaginary frequencies

H = -5199.189295

G = -5199.370294

E(M06-2X-DCM) = -5199.570313

O	-2.67683500	0.29560400	-1.19340800
O	-2.41513000	-0.97900700	1.02493900
P	-1.59406900	-0.04701900	-0.03799900
O	-1.14093700	1.13626600	0.76214600
C	-6.23016600	2.20622500	-0.11145200
C	-6.12602400	0.82020800	-0.05501800
C	-4.94947600	0.17511800	-0.46419700
C	-3.92607500	2.34605900	-0.91348900
C	-5.13967600	2.95470100	-0.55680400
C	-2.86086300	-2.23196500	0.60370300
C	-4.02611300	-2.33396400	-0.14735600
C	-4.35063100	-3.56795300	-0.73236900
C	-3.60045700	-4.70394800	-0.45179800
C	-2.49986200	-4.59911900	0.39838400
C	-2.08389500	-3.36098100	0.91331200
H	-5.20729000	4.03683600	-0.60873600
H	-1.91403700	-5.48032400	0.63866300
C	-5.13669500	-1.33256900	-0.43926300
C	-6.27030000	-1.45136000	0.63374700
H	-5.80955700	-1.42525700	1.62764800
H	-6.82816800	-2.38769100	0.54761300
H	-6.44425200	-3.84601700	-1.23797300
H	-5.36294600	-3.91643200	-2.62689000

C	-3.86309100	0.94387200	-0.85635800
H	-7.14575300	2.70552700	0.19387600
H	-3.85907700	-5.66263200	-0.89294200
C	-7.13804400	-0.19269600	0.43003000
H	-7.64917300	0.12483500	1.34523600
H	-7.91637100	-0.36550900	-0.32595900
C	-5.53000900	-3.41482900	-1.66771400
C	-5.64251600	-1.88105400	-1.81000700
H	-4.95902600	-1.53312300	-2.59187200
H	-6.65090000	-1.53390900	-2.05348600
C	-0.85449100	-3.28204600	1.75212300
C	0.37472100	-3.75018200	1.22783200
C	-0.93009900	-2.84346200	3.09764700
C	0.52575900	-4.17513000	-0.13107400
C	1.54030400	-3.80839600	2.07981400
C	0.25185400	-2.87964400	3.92761800
C	1.70399300	-4.70949900	-0.58055700
H	-0.29936500	-4.04123200	-0.81675300
C	2.75674800	-4.35513200	1.56551400
C	1.45378500	-3.35410000	3.39702800
C	2.83183600	-4.82280500	0.28247500
H	1.79984800	-4.99976300	-1.62131000
H	3.62091700	-4.39169900	2.22347300
H	2.33601900	-3.39146600	4.03093600
H	3.76303800	-5.22179100	-0.10500400
C	-2.74544100	3.15997500	-1.31279200
C	-2.17605000	4.06727500	-0.38832200
C	-2.19860700	3.02222300	-2.60860700
C	-2.66591500	4.23183800	0.94600900
C	-1.03433900	4.85777100	-0.78195400
C	-1.03615100	3.79448200	-2.97558800
C	-2.10988600	5.14572400	1.80225400
H	-3.48784200	3.61169800	1.28109500
C	-0.46548600	5.77849900	0.15035200
C	-0.49299100	4.69558500	-2.05853700
C	-0.99491200	5.93522700	1.40247300
H	-2.51122100	5.25648300	2.80599100
H	0.40116800	6.35451400	-0.16357000
H	0.38391900	5.27420300	-2.33844500
H	-0.56147400	6.64922100	2.09755300
C	-2.19266600	-2.00883600	5.01778100
H	-3.13388700	-1.68010600	5.44928800
C	-2.14689800	-2.39763100	3.70381000
H	-3.05220100	-2.38224500	3.11014800

C	-1.02333200	-2.04432400	5.82936100
H	-1.07924300	-1.73818400	6.87019200
C	0.16284700	-2.46785700	5.29349100
H	1.06605100	-2.50272000	5.89715000
C	-2.17950800	2.01187900	-4.82677700
H	-2.61149600	1.32581000	-5.54929500
C	-1.01092800	2.74657100	-5.17076200
H	-0.56065000	2.61222600	-6.14990000
C	-0.46345800	3.61940900	-4.27206900
H	0.42203200	4.19736700	-4.52459000
C	-2.75583800	2.15054800	-3.59406500
H	-3.64591200	1.58398600	-3.34990900
N	-0.46584600	-0.96958000	-0.73316900
S	-0.03193400	-0.89846000	-2.27667300
O	1.14274400	-1.75620100	-2.45989600
O	-0.01934700	0.45807000	-2.84089300
C	-1.37090800	-1.82587700	-3.22502600
F	-1.79903400	-2.88031900	-2.51164900
F	-0.84548500	-2.26766300	-4.37092400
F	-2.42717600	-1.05728000	-3.51445600
C	-0.14186400	2.05875500	4.04340800
C	0.41949000	3.08873000	3.01312200
H	0.21400200	4.09588300	3.40524400
H	-0.17779800	3.02270700	2.10542300
C	2.26049900	3.27243100	1.23385800
C	1.48002800	2.73721400	0.18824800
C	3.47632200	3.91161300	0.89940300
C	1.93750900	2.75863600	-1.12612900
H	0.53646000	2.24927000	0.39173900
C	3.90480800	3.97782800	-0.42001700
H	4.07104200	4.38210300	1.67518500
C	3.15115500	3.37522700	-1.43226900
H	1.34543800	2.27760700	-1.89803100
H	4.84464100	4.46427200	-0.65751700
H	3.51729100	3.38102200	-2.45410800
C	1.87846400	3.08648200	2.63904200
C	0.48270700	0.64704400	3.86314100
H	1.35880200	0.51509000	4.49521800
H	-0.25256600	-0.10046500	4.16790800
N	0.87730900	0.36051000	2.49144800
C	2.05661300	-0.09342500	2.06914200
N	2.12846300	-0.52406900	0.79353000
C	3.31132700	-0.61866300	0.01248700
C	4.25569600	0.41033700	-0.00291800

C	3.47611500	-1.73233800	-0.80424800
C	5.38206700	0.29359500	-0.81231000
C	4.60094600	-1.82823800	-1.62244700
H	2.72080800	-2.50089900	-0.81615400
C	5.56564600	-0.82543200	-1.62679000
H	6.44200100	-0.90779100	-2.25773500
C	4.79738500	-3.06607500	-2.45277300
C	6.37809900	1.41584500	-0.87410500
F	3.63465400	-3.54695500	-2.93202500
F	5.61693900	-2.84406600	-3.50320400
F	5.36327300	-4.06567000	-1.72343100
F	6.39366600	2.14919300	0.26185900
F	7.63353500	0.96229700	-1.08138500
F	6.10804900	2.27701500	-1.88967100
S	3.45274800	-0.09489700	3.10693200
H	4.11246200	1.29239400	0.60319400
H	1.24715900	-0.75617700	0.30943800
H	0.13563000	0.51689600	1.78985100
C	2.88307000	2.86032300	3.58185200
H	2.64535600	2.95578800	4.63649300
H	3.10428400	1.51900900	3.45659400
H	3.90384900	3.13558800	3.32074100
C	-1.66606000	1.98019600	3.81173600
H	-2.12337100	2.96749400	3.93857100
H	-2.12092700	1.29673100	4.53765200
H	-1.89881400	1.62540500	2.80591700
C	0.07730700	2.47959400	5.50843000
H	-0.38180400	1.74354300	6.17884100
H	-0.39505400	3.44815900	5.70623500
H	1.13250400	2.55285300	5.78513200

TS-EF-1S-M06-2X-DCM

l imaginary frequencies

H = -5197.135089

G = -5197.313067

E(M06-2X-DCM) = -5199.579491

O	2.46757000	-1.50172000	-0.42952500
O	2.63024100	1.01013400	-0.00943100
P	1.55156000	-0.19713700	-0.13753800
O	0.86176500	-0.27884800	1.18136900
C	5.28592500	-2.61777600	2.43346400
C	5.60146700	-1.69795200	1.44210700
C	4.66538800	-1.36867800	0.45888200
C	3.01712100	-2.78903800	1.54488100

C	4. 00603500	-3. 16684000	2. 46295200
C	3. 39835200	1. 30227300	-1. 12920200
C	4. 53453300	0. 55227500	-1. 41016200
C	5. 19199200	0. 75301700	-2. 62978200
C	4. 79200500	1. 75801200	-3. 49861600
C	3. 71151100	2. 56186800	-3. 14851800
C	2. 98185600	2. 33864400	-1. 97459300
H	3. 73883000	-3. 87876700	3. 23885700
H	3. 38924300	3. 36131600	-3. 80931800
C	5. 29903500	-0. 47848000	-0. 59182300
C	6. 41670500	0. 19251200	0. 25927300
H	5. 97362800	1. 02165200	0. 82261900
H	7. 22474600	0. 59560000	-0. 35828100
H	7. 27714800	0. 17021900	-2. 64496500
H	6. 29201800	-0. 69387800	-3. 82391300
C	3. 38370700	-1. 89126200	0. 53210500
H	6. 01754200	-2. 89639200	3. 18653300
H	5. 30759800	1. 91320800	-4. 44190100
C	6. 87420800	-0. 90938500	1. 23379200
H	7. 27626800	-0. 50905700	2. 16912900
H	7. 65742500	-1. 53547000	0. 78809300
C	6. 28740300	-0. 27218600	-2. 81464400
C	5. 94409200	-1. 31224300	-1. 73371900
H	5. 19206800	-2. 01063000	-2. 11798900
H	6. 80634300	-1. 89115100	-1. 38933800
C	1. 80744900	3. 20971800	-1. 67947900
C	0. 75030900	3. 27144800	-2. 61151000
C	1. 79959000	4. 05438300	-0. 54755600
C	0. 62083000	2. 32756200	-3. 68407800
C	-0. 26909300	4. 27201400	-2. 46861700
C	0. 73721300	5. 00991400	-0. 38430700
C	-0. 42202500	2. 39707900	-4. 55906100
H	1. 33346800	1. 51413500	-3. 75124000
C	-1. 31524400	4. 34607500	-3. 44255900
C	-0. 25404300	5. 11540700	-1. 36010800
C	-1. 39232500	3. 43868900	-4. 45574600
H	-0. 52746700	1. 63975000	-5. 32903300
H	-2. 06621700	5. 12425600	-3. 32968800
H	-1. 04125800	5. 85791000	-1. 24344300
H	-2. 20286600	3. 48874000	-5. 17656000
C	1. 61599100	-3. 27578100	1. 68955600
C	0. 90272800	-2. 96634400	2. 87099000
C	0. 99879700	-4. 01162600	0. 66026900
C	1. 46510400	-2. 20572900	3. 94950300

C	-0.45476800	-3.41111700	3.01512300
C	-0.36602500	-4.43497200	0.81039400
C	0.76433800	-1.98253600	5.09971500
H	2.47071200	-1.81372900	3.84974200
C	-1.17604800	-3.10305600	4.21248200
C	-1.05592300	-4.13075200	1.98150500
C	-0.58355700	-2.42640700	5.23625400
H	1.23265800	-1.43842300	5.91621200
H	-2.20921800	-3.43263400	4.28741800
H	-2.08987300	-4.45446500	2.09091900
H	-1.13551300	-2.21105900	6.14608900
C	2.80426800	4.87922600	1.51857200
H	3.60687900	4.85021100	2.24974200
C	2.83366000	4.03504500	0.44596300
H	3.65935600	3.34148300	0.33110000
C	1.74061700	5.81549600	1.68199800
H	1.74045000	6.48593400	2.53678600
C	0.73891800	5.87162700	0.75889600
H	-0.07399500	6.58668000	0.86029700
C	1.01719900	-4.99716600	-1.56513400
H	1.53842900	-5.21547100	-2.49218800
C	-0.34977600	-5.37769800	-1.42643200
H	-0.85917000	-5.86525900	-2.25148300
C	-1.01151600	-5.12409400	-0.26514500
H	-2.05374000	-5.40883600	-0.14503700
C	1.66990300	-4.35103000	-0.55865100
H	2.71003300	-4.06939200	-0.68307300
C	0.33533900	2.24823100	4.11237200
C	-0.17925400	3.08765900	2.90586100
H	0.12809300	4.13389400	3.06254300
H	0.35537100	2.78514100	2.00048000
C	-2.11560400	3.06256100	1.23730500
C	-1.42464700	2.27873700	0.28929400
C	-3.31641900	3.69254100	0.84681300
C	-1.93907700	2.10657700	-0.98689700
H	-0.52026700	1.74246500	0.56512100
C	-3.82252400	3.52141600	-0.43305000
H	-3.83477400	4.34837100	1.53850000
C	-3.14166100	2.71479900	-1.34421500
H	-1.41048200	1.49064600	-1.70500800
H	-4.75438600	4.00002200	-0.71577600
H	-3.54174400	2.55617500	-2.33970200
C	-1.64916100	3.15510400	2.61495400
C	-0.54630800	1.00971800	4.38126200

H	-1.46445100	1.26125800	4.91032300
H	0.01614500	0.32436000	5.02285100
N	-0.88290300	0.32444200	3.14833600
C	-2.08178800	-0.06699200	2.71793600
N	-2.08597700	-0.75871500	1.55682900
C	-3.17744600	-0.95920600	0.67195100
C	-4.13634500	0.02944500	0.43607900
C	-3.20998700	-2.14056600	-0.05991600
C	-5.12757000	-0.19483100	-0.50813400
C	-4.18465600	-2.32297700	-1.03589500
H	-2.44286300	-2.89107500	0.09161400
C	-5.16061300	-1.36626300	-1.26270000
H	-5.92822300	-1.52229400	-2.01240400
C	-4.13404800	-3.59161100	-1.83778200
C	-6.15916600	0.86290200	-0.77651300
F	-2.95784300	-3.73549000	-2.45755700
F	-5.09734700	-3.63953800	-2.76732500
F	-4.28960600	-4.67370700	-1.04895000
F	-7.37415200	0.32604700	-0.96010900
F	-5.88416200	1.56744100	-1.89079400
F	-6.25406800	1.74684900	0.22737700
S	-3.52917300	0.29640500	3.58902800
H	-4.10568200	0.96740500	0.97696100
H	-1.17305100	-1.04999600	1.18640500
H	-0.09172400	0.08497000	2.53423300
C	-2.59936600	3.23368400	3.64329300
H	-2.26375900	3.48805700	4.64421800
H	-2.95363400	1.98773700	3.69459300
H	-3.59378000	3.60050900	3.39247100
N	0.71407600	0.06909500	-1.48634200
S	-0.30012700	-1.04415900	-1.98690600
O	-1.45377200	-0.46755600	-2.66354800
O	-0.53092000	-2.08737100	-0.98314900
C	0.60749500	-1.88201000	-3.35437500
F	0.75177800	-1.03657000	-4.37550500
F	-0.09135900	-2.93525700	-3.76381600
F	1.81249000	-2.28511000	-2.96994100
C	1.75980500	1.79381300	3.75109400
H	2.38248500	2.66393400	3.51477600
H	2.21501400	1.26186700	4.59439200
H	1.77186800	1.13520800	2.87552500
C	0.41459100	3.06841600	5.40653700
H	0.78872900	2.44485800	6.22607500
H	1.10901500	3.90582500	5.28218100

H -0.55200200 3.47476200 5.71772900

TS-EF-1S-1-M06-2X-DCM

1 imaginary frequencies

H = -5197.128685

G = -5197.30906

E(M06-2X-DCM) = -5199.576558

O	1.97341400	-2.25655100	-0.33553600
O	2.87734900	0.12658900	-0.00123700
P	1.50288300	-0.70125300	-0.28706100
O	0.60333800	-0.42935600	0.87314800
C	4.03671900	-3.65272800	3.00793800
C	4.71277400	-3.06152300	1.94856000
C	4.01971600	-2.63245800	0.81406200
C	1.92679200	-3.35857800	1.81813200
C	2.65472000	-3.81026200	2.92566000
C	3.81992800	0.12696400	-1.02009800
C	4.64664700	-0.97259700	-1.18440500
C	5.42133700	-1.07386500	-2.34395900
C	5.44969000	-0.03578300	-3.26555300
C	4.72422100	1.12678800	-3.00102100
C	3.89651900	1.23058300	-1.87954800
H	2.11009800	-4.28262200	3.73845200
H	4.78299800	1.97367300	-3.67883600
C	4.98157600	-2.11182000	-0.23757500
C	6.18757200	-1.71618200	0.66746300
H	5.99508200	-0.71983400	1.08221400
H	7.12802400	-1.67616700	0.10963700
H	7.19834700	-2.29690100	-2.16997900
H	6.04133700	-2.90051200	-3.35377100
C	2.63880100	-2.75311700	0.77410200
H	4.57357500	-3.98778500	3.89079100
H	6.04408200	-0.11357200	-4.17123500
C	6.18498300	-2.75257300	1.80526800
H	6.62912300	-2.37115100	2.72932900
H	6.74555500	-3.65334600	1.52423900
C	6.12733200	-2.41236400	-2.37868700
C	5.41748600	-3.19948900	-1.25674700
H	4.51847900	-3.68303500	-1.65451800
H	6.04686200	-3.96870700	-0.79837900
C	3.23875300	2.52811100	-1.53312700
C	2.15704100	3.03588400	-2.27919700
C	3.80406200	3.29698700	-0.48998900
C	1.55338400	2.30216600	-3.35086100

C	1. 63153700	4. 34165700	-1. 97367500
C	3. 25229800	4. 58634300	-0. 17708100
C	0. 53406000	2. 84044600	-4. 08052400
H	1. 89434800	1. 29294200	-3. 55293900
C	0. 56248000	4. 86860700	-2. 76502000
C	2. 18216900	5. 07688400	-0. 92569100
C	0. 03983500	4. 14748100	-3. 79521600
H	0. 07338300	2. 24711500	-4. 86259300
H	0. 17961200	5. 85625500	-2. 52028200
H	1. 78043900	6. 06349600	-0. 69914600
H	-0. 77350600	4. 55334300	-4. 38963600
C	0. 45065500	-3. 56617100	1. 75123000
C	-0. 40492800	-2. 89133000	2. 64738900
C	-0. 07686500	-4. 47432300	0. 81216000
C	0. 06928900	-1. 92746900	3. 59716900
C	-1. 81676800	-3. 15094100	2. 60908600
C	-1. 49484900	-4. 70272000	0. 76521600
C	-0. 78952400	-1. 30526400	4. 45667000
H	1. 12857400	-1. 69087800	3. 61319600
C	-2. 68563100	-2. 45792500	3. 51043000
C	-2. 32687800	-4. 05221200	1. 67355300
C	-2. 19088600	-1. 56891300	4. 41644300
H	-0. 41008000	-0. 58855200	5. 18008100
H	-3. 75218000	-2. 65971400	3. 45106800
H	-3. 40098600	-4. 22108400	1. 62683700
H	-2. 85523400	-1. 04520400	5. 09606800
C	5. 47679400	3. 63313600	1. 25651900
H	6. 34600300	3. 28368100	1. 80486200
C	4. 94812800	2. 86459400	0. 26007700
H	5. 40292600	1. 91027800	0. 01682400
C	4. 89987200	4. 89402000	1. 58894900
H	5. 33074200	5. 48916800	2. 38831500
C	3. 82205000	5. 35235900	0. 88987000
H	3. 38458300	6. 32282400	1. 11458600
C	0. 18956800	-5. 99276700	-1. 07229800
H	0. 82874500	-6. 50200700	-1. 78695300
C	-1. 22226300	-6. 18944400	-1. 13442700
H	-1. 64003300	-6. 83553000	-1. 90002300
C	-2. 03607800	-5. 57050300	-0. 23587900
H	-3. 11445000	-5. 69853000	-0. 27160300
C	0. 74231700	-5. 17389300	-0. 13336600
H	1. 81797400	-5. 03743900	-0. 10114000
C	1. 05022000	3. 06158100	3. 06600200
C	0. 49116200	3. 78247000	1. 80033300

H	0.99299800	4.76137400	1.72493700
H	0.81382100	3.24379200	0.90505400
C	-1.67918700	3.89491000	0.43166600
C	-1.30419900	2.89623100	-0.49182600
C	-2.81566700	4.68498100	0.14244400
C	-2.04135600	2.70338700	-1.65503400
H	-0.47840800	2.21891000	-0.28432200
C	-3.54881400	4.48262200	-1.01443500
H	-3.09861900	5.49285800	0.80797400
C	-3.15967300	3.49044100	-1.91531100
H	-1.75218600	1.92085400	-2.34526100
H	-4.42178100	5.09427700	-1.21693100
H	-3.73747900	3.32233800	-2.81793900
C	-0.97535300	4.07886700	1.69735600
C	0.03330200	2.04905900	3.63586100
H	-0.73037100	2.51680600	4.25715800
H	0.57667800	1.33748100	4.27180500
N	-0.60506800	1.32566000	2.55777300
C	-1.90445300	1.07112500	2.37350800
N	-2.16572900	0.23381500	1.35507200
C	-3.38995200	0.01950800	0.68651800
C	-4.28474600	1.05164000	0.40570500
C	-3.61120800	-1.25161000	0.16829100
C	-5.41620900	0.78009100	-0.35242800
C	-4.74744500	-1.50098900	-0.59092300
H	-2.86852300	-2.02954900	0.31878700
C	-5.66921300	-0.49592000	-0.85186900
H	-6.55436500	-0.69372200	-1.44607000
C	-4.94183500	-2.89638500	-1.11161000
C	-6.33806400	1.90544300	-0.72517100
F	-3.83066900	-3.36039500	-1.69584900
F	-5.93924400	-2.97018500	-2.00086400
F	-5.23607600	-3.75791500	-0.11558200
F	-6.25031500	2.93587700	0.12795600
F	-7.61784700	1.50865900	-0.75636600
F	-6.05775300	2.39246300	-1.94912800
S	-3.12819500	1.78789100	3.35392100
H	-4.08995700	2.05878600	0.75588200
H	-1.35437800	-0.20586800	0.89931900
H	0.03034700	0.78772500	1.94955800
C	-1.71239100	4.48077400	2.82580300
H	-1.16630700	4.80130400	3.70760500
H	-2.25197200	3.36808900	3.12376800
H	-2.64982800	5.01003300	2.66359000

N	1.07857400	-0.38623000	-1.79682300
S	-0.38787300	-0.54157200	-2.34970700
O	-0.49565200	0.00473500	-3.69379800
O	-1.42485700	-0.17678700	-1.37607700
C	-0.64639800	-2.35488000	-2.55051300
F	0.40912600	-2.93346800	-3.10579300
F	-1.71388900	-2.57243800	-3.30754700
F	-0.85212200	-2.88817100	-1.34760800
C	2.30657900	2.30372900	2.61296600
H	3.03034300	2.99820400	2.17846600
H	2.78193600	1.81190400	3.46927500
H	2.08514300	1.54045600	1.85882700
C	1.46868700	4.03818800	4.17149500
H	1.85987700	3.48412600	5.03189700
H	2.26789900	4.69241800	3.80658600
H	0.64914000	4.66692500	4.53094400

TS-EF-1S-2-M06-2X-DCM

1 imaginary frequencies

H = -5197.126935

G = -5197.306524

E(M06-2X-DCM) = -5199.573542

O	1.05932000	-2.66996600	-0.26819600
O	2.79509500	-0.91857900	0.40856200
P	1.29192800	-1.06258800	-0.20652400
O	0.35074100	-0.39396200	0.73534900
C	1.73537600	-4.89371000	3.20059400
C	2.76094200	-4.64973800	2.29691400
C	2.52136800	-3.92783800	1.12518300
C	0.20362500	-3.62408700	1.78696400
C	0.46697700	-4.38750200	2.93194600
C	3.83153200	-1.31121400	-0.43173600
C	4.13227000	-2.65666400	-0.57943500
C	4.98814400	-3.05361600	-1.61204700
C	5.62805000	-2.10901600	-2.40224700
C	5.42630100	-0.75536600	-2.13501100
C	4.52251200	-0.33161700	-1.15592900
H	-0.34863700	-4.56169400	3.62810200
H	5.95712900	-0.00008800	-2.70758900
C	3.77472900	-3.85943700	0.27501700
C	4.86255600	-4.07048300	1.37209200
H	5.05413600	-3.10721400	1.85883200
H	5.80655800	-4.43335900	0.95493500
H	5.99855100	-4.94599400	-1.31607200

H	4.93115400	-4.92659600	-2.71756600
C	1.25672600	-3.40773800	0.88874200
H	1.91857300	-5.45943300	4.10955300
H	6.28924400	-2.41443300	-3.20792800
C	4.21915100	-5.03405600	2.38346300
H	4.62544200	-4.92644700	3.39335900
H	4.36484000	-6.08011300	2.08488200
C	5.04080800	-4.56422300	-1.69132500
C	3.86936500	-4.99169400	-0.78244600
H	2.93821000	-5.00926100	-1.35911000
H	4.00909200	-5.97602900	-0.32483200
C	4.38958700	1.12039500	-0.83558600
C	3.88443900	2.02810000	-1.78793300
C	4.90611600	1.59403000	0.39213700
C	3.33038500	1.59673300	-3.03694100
C	3.92917100	3.44136700	-1.51953900
C	4.90070100	3.00432500	0.66742900
C	2.91625500	2.50325800	-3.96825300
H	3.20982900	0.53452800	-3.21941800
C	3.49442400	4.35789100	-2.52821600
C	4.42007300	3.89266500	-0.29545400
C	3.02473700	3.90413700	-3.72325100
H	2.47082900	2.14821700	-4.89167400
H	3.54561200	5.42248600	-2.31368400
H	4.45080900	4.96297900	-0.09630700
H	2.69716100	4.60741300	-4.48350200
C	-1.16484900	-3.07684000	1.56725300
C	-1.68976900	-2.13389800	2.47573500
C	-1.94758500	-3.53856500	0.49239500
C	-0.91559800	-1.57598900	3.54644100
C	-3.04926600	-1.69565100	2.33558400
C	-3.28131700	-3.03188300	0.31981500
C	-1.47002400	-0.70177900	4.43643400
H	0.12750700	-1.86006000	3.63928000
C	-3.59668400	-0.78788600	3.29794100
C	-3.81077300	-2.14703300	1.25722600
C	-2.83386800	-0.29976100	4.31709300
H	-0.87065100	-0.31275400	5.25507000
H	-4.64364100	-0.51303400	3.19987700
H	-4.83342100	-1.79007500	1.14124300
H	-3.25883100	0.38827100	5.04140600
C	5.98982400	1.21727000	2.54710100
H	6.42897700	0.53915200	3.27204500
C	5.48976500	0.72803300	1.37534000

H	5.53986800	-0.33608300	1.17173000
C	5.94145500	2.61315600	2.83366700
H	6.33848400	2.98381400	3.77379400
C	5.41423600	3.47586200	1.91830400
H	5.39298400	4.54654300	2.11040400
C	-2.22132000	-4.85530600	-1.53626300
H	-1.82802500	-5.56374600	-2.25876300
C	-3.52520500	-4.30989400	-1.73084800
H	-4.10236500	-4.59425100	-2.60509100
C	-4.04154400	-3.43846200	-0.82101200
H	-5.03304000	-3.01403300	-0.95380200
C	-1.46383800	-4.49056400	-0.46327900
H	-0.47186000	-4.90948300	-0.33201500
C	1.44970900	2.69430900	3.07317500
C	1.59678700	3.43156800	1.71957100
H	2.53097900	4.01926500	1.75115900
H	1.78056300	2.70544800	0.91896100
C	0.37959200	4.58921000	-0.18100500
C	0.36251900	3.48449100	-1.05076600
C	0.15138900	5.88011200	-0.69890300
C	0.08822100	3.66795500	-2.40090600
H	0.47997600	2.47270700	-0.67352000
C	-0.07037700	6.05945700	-2.05421000
H	0.19757600	6.74157300	-0.03976900
C	-0.11526900	4.95103000	-2.90137600
H	0.04014100	2.80240100	-3.05218000
H	-0.21761900	7.05882500	-2.45071200
H	-0.30997000	5.08956400	-3.96075100
C	0.56216600	4.40462200	1.25338500
C	-0.01001600	2.28209000	3.34006800
H	-0.62245300	3.10523600	3.70497300
H	-0.01083000	1.51295600	4.12263200
N	-0.63217000	1.71981800	2.15513100
C	-1.85868300	1.96688200	1.68709500
N	-2.25605800	1.15149100	0.68518100
C	-3.55054300	0.98294400	0.15274400
C	-3.66460600	0.52969900	-1.16411100
C	-4.70062400	1.13714400	0.92675300
C	-4.91568400	0.21584900	-1.68039400
C	-5.93951300	0.81209300	0.38768800
H	-4.63359100	1.46986200	1.95476500
C	-6.06885400	0.34280400	-0.91364600
H	-7.04105900	0.09317400	-1.32162000
C	-7.12812300	0.86620100	1.30205700

C	-4.99884200	-0.30306600	-3.09076400
F	-7.08129400	-0.14162700	2.19810900
F	-8.28516700	0.75201300	0.64077700
F	-7.16740600	2.00293500	2.00775800
F	-4.20163100	0.38411000	-3.91561400
F	-6.24922600	-0.22536300	-3.57172300
F	-4.62773900	-1.59058000	-3.16640700
S	-2.79330200	3.30510500	2.24483900
H	-2.77446400	0.44319000	-1.77733700
H	-1.53709200	0.53357300	0.28995200
H	-0.16805800	0.88779100	1.76339800
C	-0.27224800	5.12657600	2.12531100
H	0.01475800	5.21807300	3.16903800
H	-1.27130500	4.34907800	2.16297100
H	-0.77801000	5.99843500	1.71077600
N	1.38866000	-0.64149900	-1.75187100
S	0.18836600	-0.07939500	-2.59172000
O	0.61759700	0.32442200	-3.92110500
O	-0.68096900	0.84602400	-1.84524400
C	-0.94600800	-1.50888000	-2.83683700
F	-0.31100600	-2.58231300	-3.27790500
F	-1.90588100	-1.17613500	-3.69436200
F	-1.50782800	-1.78366200	-1.65791300
C	2.31894300	1.43128200	2.98009700
H	3.35550400	1.70029100	2.75910200
H	2.30508300	0.89255000	3.93469700
H	1.97653400	0.74922500	2.19487400
C	1.96305800	3.52828600	4.25374300
H	1.82711300	2.97750200	5.19100500
H	3.03501900	3.71897100	4.13241800
H	1.45631300	4.49175300	4.36050900

TS-EF-1R-M06-2X-DCM

l imaginary frequencies

H = -5197.126729

G = -5197.305862

E(M06-2X-DCM) = -5199.577199

O	3.00997300	0.64135200	0.15035000
O	1.96756200	-1.67951200	-0.03440200
P	1.56846700	-0.12172400	0.15504900
O	0.72326500	0.26787700	-0.99888100
C	5.05519800	0.24328600	-3.46302900
C	5.24243300	-0.67151000	-2.43539200
C	4.59978100	-0.50123900	-1.20627700

C	3.49726300	1.48843500	-2.06007700
C	4.19817000	1.32347900	-3.26001000
C	2.76643100	-2.26934000	0.93229800
C	4.14444700	-2.11135200	0.87588100
C	4.92558700	-2.57101400	1.94045900
C	4.34784600	-3.26778800	2.99322800
C	2.97605400	-3.50918400	2.97321300
C	2.15721700	-3.00852500	1.95374100
H	4.03464800	2.04641700	-4.05435400
H	2.51066100	-4.07769100	3.77332300
C	5.04215300	-1.56701800	-0.22282200
C	5.46204800	-2.69400600	-1.21204900
H	4.56209300	-3.23864800	-1.51934400
H	6.15397500	-3.40898800	-0.75674700
H	6.97605600	-3.03209300	1.42662900
H	6.82348900	-1.77506300	2.65249800
C	3.71538200	0.55264700	-1.03990300
H	5.55472600	0.11426500	-4.41884800
H	4.95402200	-3.62681500	3.82000300
C	6.05095800	-1.94862000	-2.42455400
H	5.95620300	-2.51283900	-3.35680300
H	7.11810600	-1.73592800	-2.28146200
C	6.37054600	-2.17192900	1.73922000
C	6.27031700	-1.11997900	0.61754500
H	6.05547700	-0.13672100	1.05069200
H	7.17852800	-1.03648600	0.01261700
C	0.69605800	-3.31138900	1.96079700
C	-0.09623000	-2.90068000	3.05333400
C	0.13107400	-4.09647200	0.93096600
C	0.38657700	-1.99793800	4.05709900
C	-1.45118300	-3.36755100	3.16490700
C	-1.24307800	-4.50765900	1.02647200
C	-0.40008300	-1.62691200	5.10692700
H	1.37387100	-1.56575400	3.93603700
C	-2.22750400	-2.98874500	4.30696700
C	-1.99040700	-4.15802400	2.15035500
C	-1.72010100	-2.14595200	5.24936200
H	-0.02847800	-0.90647900	5.82810600
H	-3.23873400	-3.37983800	4.39447700
H	-3.01511900	-4.51686300	2.23599000
H	-2.32308900	-1.85135800	6.10272300
C	2.54391600	2.62185800	-1.88615300
C	1.37479900	2.68243200	-2.67099600
C	2.83184800	3.64197900	-0.95727500

C	1.00694900	1.64124700	-3.58656800
C	0.48878600	3.80536900	-2.54143900
C	1.92109700	4.74206400	-0.80917800
C	-0.13357400	1.72156900	-4.32990100
H	1.64034700	0.76307900	-3.65261100
C	-0.68550100	3.86384300	-3.36095400
C	0.78410000	4.80592400	-1.61452400
C	-0.99372200	2.85543400	-4.22347500
H	-0.40039900	0.90991300	-5.00091600
H	-1.33478200	4.73236000	-3.27415300
H	0.12977300	5.67295000	-1.53416300
H	-1.89855700	2.90297600	-4.82096500
C	0.29318600	-5.28877900	-1.19016700
H	0.87204800	-5.58834400	-2.05785000
C	0.87382600	-4.53384900	-0.21437000
H	1.91734700	-4.25452900	-0.30483900
C	-1.07413800	-5.68008100	-1.09509500
H	-1.51469100	-6.27823300	-1.88731700
C	-1.81648200	-5.30046100	-0.01812400
H	-2.86175000	-5.58539000	0.07048900
C	4.27781400	4.65221600	0.72189900
H	5.18762600	4.63519500	1.31379400
C	3.35218800	5.72289100	0.89293000
H	3.56556500	6.50613700	1.61366200
C	2.21464700	5.76656000	0.14506200
H	1.50951400	6.58740000	0.25129900
C	4.02670700	3.64985200	-0.16702800
H	4.73717500	2.83843300	-0.28478100
N	1.04144200	0.02395300	1.67559000
S	0.39811000	1.33791400	2.22540500
O	-0.55049100	1.08157500	3.30182000
O	-0.03808700	2.28949500	1.17748900
C	1.75722800	2.23949800	3.07201500
F	2.21070800	1.51211200	4.08793200
F	1.28408900	3.39149700	3.54355700
F	2.75208100	2.49084100	2.23606200
C	-2.91028900	4.91744200	0.84557200
C	-3.58511300	3.85677900	1.77369900
H	-4.17086800	4.40471200	2.52918900
H	-2.80839200	3.33175700	2.33282000
C	-4.41610400	1.44840400	1.51787900
C	-3.15496100	0.90989900	1.84114100
C	-5.52811700	0.57745200	1.46082500
C	-2.99762100	-0.44475700	2.09157400

H	-2.27814800	1.54181000	1.85362100
C	-5.37124100	-0.77353800	1.72120300
H	-6.52081200	0.96629600	1.26114100
C	-4.10724200	-1.28515400	2.03043200
H	-2.01117700	-0.83034800	2.33672400
H	-6.22870100	-1.43628000	1.67729400
H	-3.98525800	-2.34640700	2.21310800
C	-4.54130900	2.85660600	1.19065400
C	-2.67240900	4.37559900	-0.57954900
H	-3.57351300	4.43070800	-1.19150700
H	-1.91942600	5.01284700	-1.05850400
N	-2.20518200	3.00373300	-0.58361600
C	-2.64987500	1.99848500	-1.35890200
N	-1.86889600	0.90864800	-1.36637900
C	-2.22330900	-0.39612000	-1.78600500
C	-3.39795500	-1.00713100	-1.34565400
C	-1.31080400	-1.11405500	-2.55347900
C	-3.64769400	-2.32954400	-1.68989200
C	-1.58575500	-2.43486300	-2.89217100
H	-0.38226700	-0.64298800	-2.85467700
C	-2.75282900	-3.05584800	-2.47226400
H	-2.95868300	-4.08602700	-2.73649000
C	-0.59839700	-3.14575700	-3.77256900
C	-4.86118300	-3.01571900	-1.13590300
F	-0.57622100	-2.60718100	-5.00468700
F	0.64858200	-3.05740600	-3.29479300
F	-0.89029000	-4.44812700	-3.91735400
F	-5.89396200	-2.17333700	-0.98458100
F	-5.26915600	-4.02427500	-1.91707200
F	-4.62296000	-3.54883200	0.08246400
S	-4.11444200	2.08864400	-2.25718000
H	-4.10180600	-0.45340100	-0.73314000
H	-0.88288300	0.97861700	-1.05832100
H	-1.34350400	2.81433500	-0.05915700
C	-5.52034400	3.26012300	0.25592300
H	-5.73161200	4.32205300	0.17139900
H	-4.94560100	2.90913000	-0.78629700
H	-6.39803500	2.62488800	0.14219000
C	-1.56065700	5.27163100	1.49338500
H	-1.71170000	5.61966000	2.52132400
H	-1.07730600	6.08032200	0.93364100
H	-0.87573200	4.41754500	1.52427400
C	-3.72924700	6.20994800	0.73045600
H	-3.20795000	6.92534200	0.08496700

H	-3.84806300	6.67739600	1.71320900
H	-4.72408400	6.05281700	0.30470200

TS-EF-1R-1-M06-2X-DCM

l imaginary frequencies

H = -5197.130915

G = -5197.30987

E(M06-2X-DCM) = -5199.571065

O	-2.77824700	0.45025500	-1.25027700
O	-2.75179800	-0.95349900	0.88105200
P	-1.83078200	0.05339100	-0.00259700
O	-1.43911400	1.17227000	0.89222000
C	-6.33232100	2.37480800	-0.25733500
C	-6.27685600	0.98936200	-0.34427100
C	-5.09421700	0.34981300	-0.72401400
C	-3.97057100	2.50746700	-0.85206200
C	-5.18557100	3.12130100	-0.52576900
C	-3.12886600	-2.14918000	0.28535800
C	-4.22495700	-2.17753400	-0.56557300
C	-4.48906200	-3.34483400	-1.29053700
C	-3.74289000	-4.49543300	-1.07757600
C	-2.71187400	-4.47207800	-0.14045100
C	-2.36711100	-3.29894500	0.54014000
H	-5.21235700	4.20513800	-0.45635900
H	-2.13112000	-5.36955900	0.05262400
C	-5.30821600	-1.14635600	-0.84874800
C	-6.51797100	-1.32755400	0.11574800
H	-6.13652100	-1.39297800	1.14108600
H	-7.08363200	-2.24001300	-0.09450700
H	-6.54346800	-3.56631100	-1.94018200
H	-5.38281800	-3.51868200	-3.26600500
C	-3.95983800	1.11027100	-0.94843700
H	-7.25286500	2.87484200	0.02991500
H	-3.95296300	-5.40338500	-1.63546200
C	-7.34471600	-0.03748700	-0.04393800
H	-7.92536000	0.20809700	0.84993800
H	-8.05348000	-0.12000500	-0.87774100
C	-5.60792000	-3.10392200	-2.27916200
C	-5.71092400	-1.56646800	-2.28914300
H	-4.97291600	-1.15380300	-2.98621300
H	-6.70031700	-1.19313200	-2.57071300
C	-1.24244500	-3.29614200	1.52199000
C	0.06093100	-3.65181000	1.10824900
C	-1.49322900	-3.00062600	2.88054500

C	0.39439200	-3.91048300	-0.26200100
C	1.11758500	-3.74513600	2.07781200
C	-0.42096500	-3.07545000	3.83460800
C	1.65300500	-4.29577200	-0.62008400
H	-0.36557400	-3.76967100	-1.02105300
C	2.43116600	-4.13113300	1.65817300
C	0.85354100	-3.45034600	3.41453500
C	2.68914300	-4.42151400	0.35291900
H	1.88225000	-4.47397200	-1.66717800
H	3.21335500	-4.18547900	2.41084600
H	1.66192800	-3.50409900	4.14077400
H	3.68657600	-4.71102500	0.03525300
C	-2.72151600	3.29181500	-1.06569900
C	-2.17922500	4.05082600	-0.00600600
C	-2.07058700	3.24638700	-2.31517000
C	-2.76124300	4.09034300	1.30351300
C	-0.96898500	4.79383800	-0.21639900
C	-0.84415100	3.96972600	-2.50045700
C	-2.22349000	4.85824700	2.29571100
H	-3.63770900	3.48434300	1.50539100
C	-0.42543100	5.57299200	0.85416300
C	-0.33054800	4.73269400	-1.45446100
C	-1.04256400	5.62479100	2.06823500
H	-2.69101400	4.87575400	3.27597700
H	0.49000000	6.12911300	0.66713400
H	0.60064200	5.27749200	-1.59941700
H	-0.63260700	6.23318600	2.86942100
C	-2.97793800	-2.27455900	4.67651000
H	-3.96476500	-1.97495400	5.01551600
C	-2.78580300	-2.61516900	3.36982500
H	-3.62335300	-2.59135200	2.68191200
C	-1.90035600	-2.31926700	5.61105600
H	-2.07541200	-2.04674500	6.64736000
C	-0.66699300	-2.72652000	5.20139000
H	0.16449300	-2.78256500	5.89994000
C	-1.91005300	2.45916200	-4.61385100
H	-2.31121900	1.87920600	-5.43920100
C	-0.67537000	3.15215800	-4.78145100
H	-0.15015200	3.08958100	-5.72933000
C	-0.16568600	3.89016400	-3.75792000
H	0.76932900	4.43414900	-3.87003700
C	-2.58292200	2.50686100	-3.43066400
H	-3.52107500	1.97285600	-3.32268400
N	-0.63846600	-0.83057600	-0.64097400

S	-0.05319500	-0.63314500	-2.09555100
O	1.20425200	-1.37760000	-2.17375100
O	-0.08063100	0.73585500	-2.60029500
C	-1.19742200	-1.55910600	-3.22674700
F	-1.68753400	-2.63700200	-2.61400900
F	-0.52079400	-1.94652000	-4.30080200
F	-2.21218100	-0.79615900	-3.61337900
C	-0.06702500	1.48678200	3.91041900
C	0.48450600	2.59940400	2.97514800
H	0.30782800	3.56081700	3.48435200
H	-0.13826100	2.62965300	2.07631400
C	2.35360800	2.87683800	1.21302700
C	1.58933800	2.44789700	0.10998700
C	3.59275200	3.50587400	0.96750500
C	2.09995800	2.55009600	-1.18074700
H	0.60154900	2.01140000	0.24755600
C	4.07765900	3.64646600	-0.32338400
H	4.16853700	3.91031900	1.79315500
C	3.34625600	3.13655400	-1.39604700
H	1.51152100	2.16742000	-2.00931300
H	5.03566900	4.12671500	-0.48959400
H	3.74444600	3.20608700	-2.40397400
C	1.93769300	2.61894900	2.59684800
C	0.14136100	0.04934300	3.33053200
H	0.66438700	-0.57627300	4.05499400
H	-0.83870400	-0.39995400	3.13829500
N	0.87100000	-0.04616700	2.07535100
C	2.09145300	-0.52666400	1.85760200
N	2.36654400	-0.86561200	0.57705900
C	3.62960000	-0.81637500	-0.05223100
C	4.55089100	0.18696900	0.25207500
C	3.91609800	-1.73273800	-1.05855500
C	5.76411200	0.23061500	-0.41739700
C	5.14382000	-1.67869200	-1.70968800
H	3.17464500	-2.47023600	-1.33574100
C	6.08506300	-0.70854900	-1.39509100
H	7.04564400	-0.68079500	-1.89840100
C	5.42140200	-2.68537600	-2.79059400
C	6.73124900	1.34537000	-0.14245700
F	4.92087100	-2.30317000	-3.97117700
F	6.73717200	-2.87813000	-2.96060700
F	4.87095300	-3.87637700	-2.49818800
F	6.72882700	2.25256100	-1.13644100
F	6.44110300	2.00563000	0.98972700

F	7.98902700	0.89590800	-0.03907100
S	3.24228000	-0.66758700	3.13435400
H	4.31710800	0.93529900	0.99849600
H	1.57527900	-1.09734700	-0.03349500
H	0.30636500	0.15536400	1.25102500
C	2.92915000	2.35532600	3.54670500
H	2.69052500	2.48146800	4.59732600
H	2.98047800	1.03800100	3.44363300
H	3.96489300	2.56125900	3.28255100
C	-1.57897600	1.74589100	4.02813700
H	-1.76643900	2.70271600	4.52911900
H	-2.04377200	0.95203000	4.62419500
H	-2.04654200	1.76129700	3.04048300
C	0.50538400	1.50258300	5.33958700
H	-0.13073100	0.87849100	5.97755600
H	0.50919700	2.51428200	5.76165800
H	1.51276900	1.08380700	5.40115400

TS-EF-1R-2-M06-2X-DCM

l imaginary frequencies

H = -5197.128413

G = -5197.307488

E(M06-2X-DCM) = -5199.575229

O	-3.16298400	0.52739800	-0.93993800
O	-2.13736400	-1.49351800	0.25986900
P	-1.73032800	-0.14452100	-0.56689100
O	-0.93536500	0.66758100	0.40487500
C	-5.55537600	1.49428400	2.32901700
C	-5.60399500	0.22447100	1.76676300
C	-4.85035500	-0.07704400	0.62967100
C	-3.93696400	2.17882300	0.63516500
C	-4.74786100	2.46614200	1.74067700
C	-2.82895700	-2.47509400	-0.43542500
C	-4.19832100	-2.35675100	-0.59445000
C	-4.86227700	-3.23619700	-1.45455300
C	-4.17499900	-4.27669400	-2.06584500
C	-2.81938100	-4.45558600	-1.78326400
C	-2.12291500	-3.56116600	-0.96642500
H	-4.72565200	3.47360000	2.14694500
H	-2.27904800	-5.29805500	-2.20553000
C	-5.19530800	-1.46115700	0.11387700
C	-5.69783100	-2.12669800	1.42896800
H	-4.82555400	-2.48075000	1.99125500
H	-6.34801700	-2.98544100	1.23622200

H	-6.95771400	-3.53785100	-1.00783800
H	-6.67255200	-2.84614500	-2.60317700
C	-3.98605200	0.87797000	0.11530800
H	-6.14788500	1.73501100	3.20716200
H	-4.68566400	-4.95814500	-2.74002200
C	-6.38792100	-0.99074400	2.20732800
H	-6.35901300	-1.13977800	3.29088600
H	-7.44356300	-0.89689200	1.92241400
C	-6.31937100	-2.84288400	-1.56798000
C	-6.33799200	-1.43351700	-0.93974900
H	-6.08835800	-0.68680300	-1.70180700
H	-7.30280300	-1.16383800	-0.49889400
C	-0.71678400	-3.80847900	-0.53364700
C	0.36820900	-3.69585400	-1.42255200
C	-0.50482300	-4.21383400	0.80333300
C	0.20308700	-3.29881400	-2.78904600
C	1.69954000	-3.98070500	-0.95508300
C	0.83346900	-4.44046700	1.27158500
C	1.27198300	-3.23645100	-3.63447800
H	-0.78264700	-3.00438700	-3.13362900
C	2.79036300	-3.91825400	-1.88027900
C	1.90382700	-4.31180000	0.38407900
C	2.58319900	-3.57058600	-3.18249500
H	1.12708800	-2.89197700	-4.65234400
H	3.79154200	-4.13483300	-1.51524600
H	2.91519100	-4.49399200	0.74171700
H	3.42090200	-3.50787300	-3.87008100
C	-3.08861500	3.23001400	0.00359000
C	-2.07483000	3.86832600	0.74721700
C	-3.33805900	3.61696200	-1.33145800
C	-1.77784000	3.52800800	2.10740000
C	-1.29307900	4.90901600	0.13853200
C	-2.53383700	4.64357100	-1.93389200
C	-0.81419600	4.19172800	2.81027500
H	-2.33518800	2.72201500	2.57465900
C	-0.27934800	5.56740800	0.90582700
C	-1.53579400	5.26559100	-1.18601200
C	-0.04911500	5.23090500	2.20500600
H	-0.61162700	3.91798100	3.84264400
H	0.30152400	6.34818500	0.42137000
H	-0.93508500	6.04745200	-1.64627700
H	0.72391300	5.73389500	2.77785400
C	-1.34239400	-4.85779600	3.00515400
H	-2.17601000	-5.05022000	3.67449600

C	-1.58185900	-4.45221400	1.72271300
H	-2.60340500	-4.32906400	1.37793200
C	-0.00866600	-5.03807800	3.47596500
H	0.16241900	-5.34995300	4.50177000
C	1.04297100	-4.83144400	2.63276000
H	2.06651200	-4.96805200	2.97104300
C	-4.58302300	3.42810300	-3.41748900
H	-5.37919300	2.97353500	-3.99862800
C	-3.75730800	4.42069400	-4.02084600
H	-3.92577200	4.70312800	-5.05517700
C	-2.76912600	5.01304900	-3.29560200
H	-2.13658300	5.77984500	-3.73501800
C	-4.38400300	3.04317700	-2.12494600
H	-5.02928400	2.29165100	-1.68364000
N	-1.16654600	-0.57587400	-1.99433700
S	0.01141500	0.12606600	-2.76819300
O	0.12372000	-0.38675200	-4.12011400
O	1.24323600	0.25639700	-1.96976900
C	-0.51718700	1.88313800	-2.95988800
F	-1.74640800	1.95227300	-3.45004300
F	0.31672300	2.52295900	-3.77031500
F	-0.49739900	2.48007600	-1.76549000
C	-0.77544200	-0.49960800	3.93862100
C	-0.12638300	0.91501800	3.86433100
H	-0.49310900	1.49524000	4.72792700
H	-0.51684400	1.42008900	2.97964700
C	2.01770000	1.98049900	2.94288400
C	1.48816700	2.18959400	1.65264600
C	3.23907900	2.60595800	3.27887800
C	2.18752300	2.93964800	0.71612300
H	0.55708900	1.72762300	1.34180800
C	3.91398200	3.38408200	2.35124900
H	3.64387600	2.50848200	4.28083100
C	3.40041900	3.53285100	1.06033900
H	1.77649800	3.03928500	-0.28335800
H	4.85553300	3.85108100	2.61919100
H	3.95647400	4.10570300	0.32490800
C	1.36498600	1.07216000	3.88232300
C	0.03689900	-1.54125500	3.12975400
H	0.78888100	-2.02926700	3.75190600
H	-0.65015900	-2.31718500	2.77432100
N	0.71171000	-0.96459300	1.98189300
C	1.99235900	-1.11786900	1.63315800
N	2.30895800	-0.67766000	0.40182900

C	3.60799800	-0.39951400	-0.08608800
C	4.50905800	0.36552600	0.65301100
C	3.93980500	-0.82234700	-1.36697000
C	5.74951800	0.67212300	0.11211200
C	5.20035700	-0.52952400	-1.87923300
H	3.21315000	-1.36907600	-1.95692100
C	6.11810500	0.21628300	-1.15238900
H	7.09618800	0.44425600	-1.56092000
C	5.55850600	-1.10646100	-3.21921800
C	6.66640500	1.58598300	0.87116700
F	4.58162400	-0.92647700	-4.11420200
F	6.67983800	-0.56850600	-3.71693400
F	5.76040600	-2.43542000	-3.13182700
F	6.49461200	1.48405500	2.19783300
F	7.95511900	1.33952500	0.60500800
F	6.44693100	2.87876700	0.55620000
S	3.17047400	-1.78048000	2.70381800
H	4.23612500	0.72226700	1.63936900
H	1.56295900	-0.44601300	-0.26655600
H	0.10224200	-0.45633100	1.32063700
C	2.16101900	0.30623200	4.75715500
H	1.67163800	-0.17277700	5.59968400
H	2.49609400	-0.62308100	3.98244600
H	3.16707500	0.66606700	4.96956700
C	-2.18952100	-0.34192600	3.35013900
H	-2.77737500	0.36648200	3.94731100
H	-2.71132300	-1.30584000	3.35433900
H	-2.15878100	0.02412100	2.32073500
C	-0.93346800	-1.04318700	5.36532100
H	-1.44318000	-2.01279800	5.32642900
H	-1.54491000	-0.36889800	5.97403600
H	0.01855600	-1.20450100	5.87712700

TS-EF-1S-蠅B97X-D

1 imaginary frequencies

H = -5197.532778

G = -5197.712137

E(M06-2X-DCM) = -5199.581798

O	2.23985400	-1.85196700	-0.24187300
O	2.52629500	0.68879100	0.04009200
P	1.39823300	-0.47227300	-0.13643800
O	0.59993200	-0.42008600	1.12661500
C	4.43931000	-2.89529200	3.13375600
C	4.97895800	-2.07057900	2.15687000

C	4.25546800	-1.78294300	0.99947400
C	2.37354300	-3.06851400	1.84481400
C	3.15556600	-3.40536000	2.95587400
C	3.48020300	0.83762400	-0.95406600
C	4.57182000	-0.02052400	-1.00005700
C	5.42378300	0.02960700	-2.10708100
C	5.25523100	0.99045300	-3.09258400
C	4.22819400	1.91905400	-2.96019000
C	3.31833100	1.85608000	-1.90048400
H	2.72235000	-4.05463200	3.71108200
H	4.10076700	2.70096900	-3.70280100
C	5.11492400	-1.01748000	0.01368100
C	6.10807500	-0.33087700	0.99808800
H	5.63213400	0.57164700	1.39925100
H	7.04015900	-0.03046900	0.51021900
H	7.43702400	-0.67945200	-1.75972300
H	6.56983500	-1.59394800	-2.99179200
C	2.95654400	-2.24375100	0.87373900
H	5.00321700	-3.13877900	4.02986500
H	5.91886900	1.02673300	-3.95169900
C	6.30999200	-1.35712800	2.12895900
H	6.55551700	-0.88784500	3.08690100
H	7.12565800	-2.05331800	1.89442200
C	6.45083900	-1.07505600	-2.03562700
C	5.88123500	-1.98425300	-0.93330600
H	5.16115100	-2.68687400	-1.36731400
H	6.64511100	-2.56469700	-0.40716400
C	2.26249900	2.90562200	-1.78885500
C	1.24485900	2.99004800	-2.75703400
C	2.36849700	3.89195600	-0.78523300
C	1.05227900	1.97882100	-3.75233100
C	0.34473000	4.10757500	-2.74767200
C	1.44072700	4.98725600	-0.76674600
C	0.05260100	2.07892000	-4.67123700
H	1.68345100	1.10001000	-3.73239900
C	-0.66824000	4.19370300	-3.75365000
C	0.45776800	5.07308100	-1.75158300
C	-0.81190700	3.21142100	-4.68529400
H	-0.10319300	1.27512300	-5.38259300
H	-1.33631200	5.05094800	-3.73907200
H	-0.23626500	5.91072000	-1.74053000
H	-1.59541800	3.27688700	-5.43449100
C	0.96493100	-3.54382100	1.72837000
C	0.01502100	-3.14827900	2.69555800

C	0.58088000	-4.36717700	0.65253800
C	0.32455900	-2.27039100	3.78558100
C	-1.33828600	-3.61110500	2.58618200
C	-0.78577800	-4.78508200	0.53151500
C	-0.62104000	-1.91923800	4.70407000
H	1.32878200	-1.86948600	3.86671600
C	-2.30421700	-3.20395300	3.55920200
C	-1.70437700	-4.41881300	1.51007700
C	-1.96051000	-2.38731500	4.59341100
H	-0.35728900	-1.26135300	5.52778800
H	-3.32595300	-3.55730600	3.44662300
H	-2.73859700	-4.74043800	1.41470600
H	-2.70163700	-2.07880500	5.32405800
C	3.49840000	4.86542600	1.14634400
H	4.29915100	4.83598000	1.87997300
C	3.39934500	3.87762100	0.21000200
H	4.12284500	3.06955400	0.20302000
C	2.57042900	5.94590200	1.16455700
H	2.66868700	6.72789800	1.91207700
C	1.57089900	5.99663600	0.23870600
H	0.85968500	6.81904000	0.23504400
C	1.07888900	-5.54457400	-1.41772200
H	1.79270600	-5.85051800	-2.17656300
C	-0.28995600	-5.91060600	-1.55877800
H	-0.60717100	-6.47616700	-2.42941800
C	-1.19063800	-5.55203400	-0.60494200
H	-2.24010700	-5.81401800	-0.69971300
C	1.49960800	-4.80726200	-0.35288500
H	2.54672000	-4.54060800	-0.26457300
C	0.86350400	2.65516500	3.71380300
C	0.38674900	3.40396900	2.43269800
H	0.85980400	4.39636700	2.42248100
H	0.80500900	2.90446400	1.55691100
C	-1.62407900	3.47057300	0.85330800
C	-1.13776100	2.45263500	0.01341600
C	-2.71291300	4.24290000	0.40524800
C	-1.74466200	2.18636100	-1.20362200
H	-0.32033200	1.81700400	0.33239800
C	-3.30723900	3.98584900	-0.82105900
H	-3.07455100	5.07259800	1.00410000
C	-2.83315600	2.94690400	-1.61850500
H	-1.37162700	1.38482600	-1.83080500
H	-4.14978700	4.58575500	-1.14886400
H	-3.30661700	2.72657300	-2.56841100

C	-1.07389800	3.66411700	2.19647900
C	-0.16497900	1.59794600	4.17949000
H	-0.97743900	2.03854400	4.75625600
H	0.34300700	0.88102200	4.83675600
N	-0.71327700	0.88232200	3.05028600
C	-1.98214100	0.61834200	2.74801200
N	-2.15271700	-0.21190700	1.70268100
C	-3.28481400	-0.39633200	0.87480500
C	-4.16858100	0.63712700	0.56360500
C	-3.42259400	-1.63689000	0.26462100
C	-5.20605900	0.39848800	-0.32470200
C	-4.45861500	-1.85339900	-0.63801500
H	-2.69992400	-2.41888100	0.46619200
C	-5.36437000	-0.84592200	-0.93138400
H	-6.17673000	-1.01990900	-1.62669600
C	-4.56380900	-3.20526700	-1.29393300
C	-6.14373100	1.51194800	-0.70326400
F	-3.53949600	-3.44779800	-2.11509800
F	-5.69629700	-3.33127600	-2.00564800
F	-4.56789800	-4.19335700	-0.37040100
F	-7.41876800	1.08979000	-0.74456800
F	-5.86307400	2.00371800	-1.92707100
F	-6.08805800	2.54316300	0.15490000
S	-3.29059500	1.32202100	3.63395200
H	-4.03839200	1.62083700	0.99369900
H	-1.29177100	-0.64400300	1.34979100
H	-0.02425900	0.44150000	2.42665500
C	-1.93775300	4.02502700	3.22757500
H	-1.52122200	4.34293800	4.17912300
H	-2.50846800	2.82580400	3.48115700
H	-2.88765600	4.49204700	2.96960900
N	0.70986100	-0.23674400	-1.55535500
S	-0.35128400	-1.24614600	-2.16997300
O	-1.34369700	-0.53270500	-2.96270000
O	-0.81149200	-2.25983200	-1.22303600
C	0.63960400	-2.16836300	-3.43745100
F	1.01918900	-1.33738200	-4.41343600
F	-0.10780600	-3.13197700	-3.96709700
F	1.72930900	-2.70966700	-2.90324400
C	2.18430300	1.95254000	3.34671800
H	2.90298400	2.67933500	2.95405400
H	2.62393500	1.47529700	4.23026900
H	2.04641100	1.18920800	2.57416500
C	1.14048200	3.61259200	4.88152000

H	1.47669200	3.05456700	5.76307700
H	1.93301900	4.31914600	4.61269700
H	0.25964300	4.19174700	5.17505700

TS-EF-1S-1-蠅B97X-D

l imaginary frequencies

H = -5197.524509

G = -5197.706545

E(M06-2X-DCM) = -5199.574667

O	-0.93413500	-2.64299400	0.16377100
O	-2.69568800	-0.84814000	-0.35790700
P	-1.20511500	-1.04482500	0.27482900
O	-0.27063800	-0.25888400	-0.58775100
C	-1.60074600	-4.71236200	-3.39299000
C	-2.63270200	-4.48746800	-2.49375100
C	-2.39839500	-3.81921000	-1.29085100
C	-0.07240600	-3.51485400	-1.91824400
C	-0.33002800	-4.23732300	-3.08956500
C	-3.75957200	-1.29962700	0.41170900
C	-4.03848600	-2.65531300	0.47750800
C	-4.90891400	-3.12262000	1.46505600
C	-5.60003400	-2.23425600	2.27524000
C	-5.43636000	-0.86625100	2.06885400
C	-4.51104000	-0.37430800	1.14519300
H	0.49086800	-4.40194600	-3.78124700
H	-6.01332500	-0.15393400	2.65112400
C	-3.65507600	-3.80135100	-0.44116900
C	-4.73824100	-3.95388600	-1.55454600
H	-4.93427800	-2.96509000	-1.98542500
H	-5.68367500	-4.34296200	-1.16567500
H	-5.87153200	-5.02513400	1.08173400
H	-4.80493700	-5.04040800	2.48365400
C	-1.13293500	-3.31575300	-1.02520500
H	-1.77966300	-5.24315700	-4.32372200
H	-6.27547600	-2.59370700	3.04610500
C	-4.09025600	-4.85686900	-2.61529500
H	-4.48739600	-4.68524800	-3.62065100
H	-4.24514900	-5.91890700	-2.38404100
C	-4.92381400	-4.63470100	1.47423900
C	-3.74042500	-4.99218100	0.55133900
H	-2.81229400	-5.03083300	1.13183200
H	-3.86303100	-5.95270300	0.04122800
C	-4.42168900	1.09313800	0.88342400
C	-3.87108100	1.97219800	1.83413400

C	-5.00251400	1.59932200	-0.29928000
C	-3.27548500	1.50549700	3.04885300
C	-3.91062500	3.38946300	1.59952400
C	-5.00796500	3.01424500	-0.53769000
C	-2.78679500	2.38179000	3.97103900
H	-3.18993700	0.43919300	3.21875900
C	-3.39380700	4.27451500	2.59618900
C	-4.46736900	3.87416000	0.41802600
C	-2.86191300	3.78664800	3.75027500
H	-2.31402300	1.99670900	4.86818000
H	-3.42845100	5.34423600	2.40691800
H	-4.49325100	4.94854000	0.24393400
H	-2.46790500	4.46747900	4.49896300
C	1.30093600	-2.98862700	-1.67609300
C	1.83682800	-2.02701700	-2.55697900
C	2.08529400	-3.50315600	-0.62659700
C	1.07770500	-1.44200700	-3.62363800
C	3.20018300	-1.60934800	-2.40410400
C	3.42126500	-3.01459500	-0.43596700
C	1.64844200	-0.56568300	-4.49929600
H	0.03218900	-1.71018800	-3.72991100
C	3.76378500	-0.69681600	-3.35094100
C	3.95318700	-2.09454600	-1.33658100
C	3.01543100	-0.18769300	-4.36897100
H	1.05819200	-0.15306000	-5.31300400
H	4.81044100	-0.42835900	-3.23978900
H	4.97657800	-1.74827300	-1.20836000
H	3.45405300	0.50373700	-5.08177100
C	-6.17121500	1.27348400	-2.41599500
H	-6.63691500	0.61252600	-3.14066500
C	-5.62662700	0.75734300	-1.27708200
H	-5.66481900	-0.31159800	-1.09917500
C	-6.13468900	2.67454400	-2.66803000
H	-6.56755500	3.06832500	-3.58285300
C	-5.57458000	3.51527500	-1.75268100
H	-5.56104100	4.58950900	-1.92263600
C	2.38097200	-4.96438500	1.29626700
H	1.99464100	-5.72422900	1.96875800
C	3.68705500	-4.43903800	1.51180000
H	4.27636300	-4.79260900	2.35213600
C	4.19144400	-3.49910600	0.66653500
H	5.18527600	-3.08876400	0.81964800
C	1.60933800	-4.51505200	0.26742600
H	0.61443200	-4.92032700	0.12123600

C	-1.60493900	2.64687200	-3.03115200
C	-1.67645100	3.30317000	-1.63002000
H	-2.65184800	3.80579100	-1.53515900
H	-1.72233900	2.52280200	-0.86253800
C	-0.42851900	4.50160100	0.23203000
C	-0.21887200	3.39684800	1.07308200
C	-0.31112000	5.80019800	0.76166500
C	0.14550300	3.59667900	2.39893700
H	-0.27546300	2.37903300	0.69713800
C	0.00571600	5.98947100	2.09679700
H	-0.50882000	6.65953900	0.12782100
C	0.25360500	4.88543000	2.90992500
H	0.33911700	2.72942600	3.01762900
H	0.07078800	6.99526700	2.50002000
H	0.52570400	5.02982100	3.95125800
C	-0.68078700	4.33277400	-1.19942300
C	-0.15198800	2.28077200	-3.40503800
H	0.41761200	3.13187900	-3.77479500
H	-0.17606400	1.54042600	-4.21359200
N	0.55116400	1.69566500	-2.28340300
C	1.74968800	2.00953500	-1.79365900
N	2.17970000	1.19989700	-0.80490400
C	3.46001800	1.09756600	-0.22344200
C	3.52745100	0.65115700	1.09588200
C	4.62873400	1.30249200	-0.94884800
C	4.76441000	0.39088700	1.66957300
C	5.85724100	1.03204600	-0.35768900
H	4.58625600	1.62929200	-1.97899300
C	5.94067500	0.57009500	0.94918500
H	6.90285100	0.36090900	1.40057100
C	7.08860400	1.12477400	-1.21370900
C	4.82587400	-0.14711100	3.07591700
F	7.18297700	0.04703900	-2.02716500
F	8.21502000	1.16776800	-0.48942000
F	7.07042100	2.20459300	-2.00886300
F	3.82411600	0.31516900	3.83163600
F	5.98127700	0.18721900	3.67975900
F	4.75364000	-1.48991700	3.09085200
S	2.61568600	3.41211100	-2.31496000
H	2.61158700	0.51504700	1.66273300
H	1.49871100	0.50426100	-0.48199500
H	0.11218500	0.86711900	-1.86669300
C	0.06999600	5.11369500	-2.08139800
H	-0.24810600	5.21033000	-3.11505900

H	1.13597900	4.36121200	-2.17856100
H	0.56787100	5.99214800	-1.67063000
N	-1.33374400	-0.80286600	1.84041300
S	-0.23037500	-0.40011000	2.87997400
O	-0.80932700	-0.24476200	4.20372400
O	0.68088300	0.64791900	2.39950500
C	0.89054900	-1.87313600	2.99574200
F	0.20020100	-3.00360700	3.08153700
F	1.67893400	-1.76287100	4.05847400
F	1.65169900	-1.90948300	1.89873600
C	-2.44319800	1.35917700	-2.96271200
H	-3.47499300	1.58697600	-2.68496400
H	-2.46096200	0.86665000	-3.94202300
H	-2.05876700	0.64783200	-2.22673000
C	-2.20885900	3.53084500	-4.13233500
H	-2.13459500	3.02830900	-5.10357600
H	-3.27133100	3.70266200	-3.92840300
H	-1.72163100	4.50530800	-4.22918700

TS-EF-1R-蠅B97X-D

l imaginary frequencies

H = -5197.524857

G = - 5197.706299

E(M06-2X-DCM) = -5199.576684

O	3.04748500	0.32108600	0.09236100
O	1.74823100	-1.88016900	-0.02291700
P	1.53590300	-0.28511600	0.14712300
O	0.71103100	0.17021500	-0.99993300
C	5.02967200	-0.31395000	-3.51745800
C	5.10019400	-1.24662600	-2.49303400
C	4.48707100	-0.99959700	-1.26359300
C	3.63316200	1.10757200	-2.11502600
C	4.31494500	0.86262000	-3.31138900
C	2.49833300	-2.55973100	0.92004600
C	3.88358700	-2.54717900	0.83771700
C	4.63011800	-3.09223100	1.88485200
C	4.00397100	-3.74518300	2.93633800
C	2.61661000	-3.85158200	2.93487300
C	1.83618400	-3.25052100	1.94154300
H	4.24484300	1.60141900	-4.10439600
H	2.11180800	-4.38548300	3.73440600
C	4.81656200	-2.10347500	-0.27730300
C	5.09259000	-3.27657200	-1.26505200
H	4.13350100	-3.72020800	-1.55548500

H	5.70539500	-4.06434800	-0.81685100
H	6.62256900	-3.75283000	1.35950200
H	6.60004400	-2.47978500	2.57765600
C	3.73136200	0.14976900	-1.09784300
H	5.51085200	-0.50059700	-4.47329100
H	4.58430700	-4.17542400	3.74762100
C	5.74599600	-2.61139900	-2.48960600
H	5.56546800	-3.16286800	-3.41748600
H	6.83427300	-2.53216500	-2.36798700
C	6.10352400	-2.83668200	1.66984700
C	6.09755900	-1.78567500	0.54444300
H	5.99662100	-0.78241600	0.97332400
H	7.00230600	-1.80091800	-0.07104000
C	0.35159700	-3.39293800	1.98286300
C	-0.36621100	-2.89040600	3.08695000
C	-0.31856500	-4.11030400	0.96887700
C	0.23735300	-2.05578100	4.08274500
C	-1.76270400	-3.19357900	3.22343800
C	-1.73019900	-4.34438400	1.08220200
C	-0.47788300	-1.60008400	5.14872300
H	1.26587300	-1.74367700	3.94821200
C	-2.46627700	-2.73103100	4.38076900
C	-2.41019600	-3.90793700	2.21730600
C	-1.84535600	-1.95945000	5.31515300
H	-0.00832500	-0.93479500	5.86581900
H	-3.51571600	-2.99567400	4.48691200
H	-3.46966900	-4.13588600	2.31867100
H	-2.39375600	-1.59883600	6.18029200
C	2.81653400	2.34633100	-1.96187500
C	1.65850300	2.51850000	-2.74548600
C	3.22307500	3.35158100	-1.06374900
C	1.16817600	1.50318500	-3.63031200
C	0.91231100	3.73935600	-2.64938600
C	2.45488900	4.55751900	-0.95529200
C	0.03849800	1.69158100	-4.36894100
H	1.69698800	0.55848200	-3.67989600
C	-0.26000200	3.90437400	-3.45432400
C	1.33440200	4.73077500	-1.76482100
C	-0.68906200	2.91362800	-4.28414500
H	-0.32291100	0.89779400	-5.01652400
H	-0.81224900	4.83823000	-3.38017400
H	0.78690400	5.67048000	-1.71358600
H	-1.59222600	3.04431300	-4.87177800
C	-0.33308900	-5.31319400	-1.15116300

H	0.19461600	-5.68878000	-2.02168600
C	0.34955700	-4.64353000	-0.18061600
H	1.42020500	-4.50838700	-0.27884300
C	-1.73783700	-5.51624900	-1.04539900
H	-2.26273100	-6.04538400	-1.83488300
C	-2.41208100	-5.04943100	0.04105000
H	-3.48442700	-5.19497500	0.13610000
C	4.76388900	4.22024000	0.60906800
H	5.65637100	4.10424500	1.21641800
C	3.98114600	5.40280200	0.73517700
H	4.28259200	6.17347300	1.43825800
C	2.86681100	5.56650400	-0.02986300
H	2.26854200	6.47125900	0.04690700
C	4.40054300	3.23459500	-0.25842000
H	5.00594700	2.33898100	-0.34327900
N	1.05768700	-0.05268700	1.66669000
S	0.65169200	1.33797800	2.25229100
O	-0.34700200	1.22050000	3.30775900
O	0.40246600	2.37925600	1.23132600
C	2.14843900	1.94257000	3.15822900
F	2.42592300	1.10914200	4.15983500
F	1.89423000	3.15048600	3.66135800
F	3.20287400	2.02069800	2.35991900
C	-2.26189400	5.18122800	0.91436600
C	-3.09933300	4.24538700	1.84593600
H	-3.60842300	4.88576500	2.58231400
H	-2.41137100	3.63120800	2.42809600
C	-4.24246900	1.96088800	1.63239400
C	-3.06621000	1.26287600	1.95682400
C	-5.45501400	1.24097000	1.58143700
C	-3.08381100	-0.10243100	2.19094200
H	-2.11271400	1.76905200	1.99173600
C	-5.47467300	-0.12068100	1.83403400
H	-6.39054900	1.75308400	1.38304700
C	-4.28811900	-0.79505700	2.12651000
H	-2.15410900	-0.61122000	2.42195600
H	-6.41173600	-0.66475500	1.78930600
H	-4.30120400	-1.86530000	2.29368000
C	-4.18054900	3.37144700	1.27299500
C	-2.04665200	4.58235700	-0.49474600
H	-2.90412000	4.77025600	-1.14110100
H	-1.18809800	5.08885200	-0.94700400
N	-1.79147200	3.15601800	-0.49555000
C	-2.39289700	2.23539200	-1.26532800

N	-1.79710100	1.03805400	-1.29415500
C	-2.33345100	-0.18937400	-1.74951700
C	-3.56859900	-0.65888000	-1.31027400
C	-1.53101600	-0.98746100	-2.55674000
C	-3.99467100	-1.92297700	-1.69882700
C	-1.97233200	-2.24903700	-2.93649900
H	-0.55558100	-0.62517500	-2.85566200
C	-3.20502200	-2.72682400	-2.51643300
H	-3.54275400	-3.71193400	-2.81103500
C	-1.09535000	-3.04884000	-3.85983100
C	-5.29156300	-2.45927400	-1.16169900
F	-1.05125500	-2.48925600	-5.08568000
F	0.16957300	-3.10861600	-3.41972300
F	-1.53248600	-4.31007600	-4.01875600
F	-6.21218300	-1.49305300	-1.00485700
F	-5.82123600	-3.39637100	-1.96315800
F	-5.13268200	-3.03646400	0.05114800
S	-3.84316500	2.55547500	-2.14488300
H	-4.18357900	-0.04514400	-0.66373900
H	-0.80050000	0.95593400	-1.02466100
H	-0.96254900	2.84545900	0.02331900
C	-5.08294300	3.87329100	0.32455100
H	-5.15318500	4.94994900	0.20018100
H	-4.52986800	3.41878300	-0.73822900
H	-6.02785900	3.34891900	0.18634900
C	-0.90199400	5.38872200	1.60668100
H	-1.04423300	5.78820900	2.61741500
H	-0.29741600	6.10990700	1.04482100
H	-0.33006500	4.45970500	1.68560900
C	-2.91039400	6.56322900	0.73400100
H	-2.28065400	7.19328200	0.09553600
H	-3.01187000	7.07041900	1.69935100
H	-3.89933700	6.51726100	0.26863700

TS-EF-1R-1-蠅B97X-D

1 imaginary frequencies

H = -5197.526414

G = -5197.705988

E(M06-2X-DCM) = -5199.576092

O	-3.16546700	0.52507900	-0.97603600
O	-2.12385600	-1.50399300	0.21088700
P	-1.73275700	-0.15374800	-0.62319600
O	-0.92310900	0.64782200	0.34446300
C	-5.63440700	1.50258500	2.22956800

C	-5.64328000	0.22354300	1.69165300
C	-4.86654000	-0.08198000	0.57287900
C	-3.99185900	2.18627600	0.56191100
C	-4.83646500	2.47817300	1.63907900
C	-2.82057000	-2.50578200	-0.43998900
C	-4.18758700	-2.38444800	-0.61341300
C	-4.84978900	-3.28922100	-1.44545800
C	-4.17102300	-4.36705600	-1.99628700
C	-2.82704400	-4.55683400	-1.67649400
C	-2.12887100	-3.63310700	-0.89594300
H	-4.84465700	3.49241300	2.02733100
H	-2.29670700	-5.43057500	-2.04350900
C	-5.19052800	-1.47641700	0.07056900
C	-5.69386300	-2.13068600	1.39261500
H	-4.82164700	-2.46492400	1.96708200
H	-6.32952400	-3.00233400	1.21066100
H	-6.95664800	-3.57154500	-1.04170700
H	-6.62954300	-2.90614400	-2.63991600
C	-4.00458400	0.87655700	0.06231100
H	-6.24971300	1.74751200	3.09075200
H	-4.68178800	-5.07184100	-2.64607100
C	-6.40739400	-0.99591500	2.14792800
H	-6.37972000	-1.12696700	3.23432800
H	-7.46419700	-0.92682800	1.85907700
C	-6.29985800	-2.88901900	-1.59650900
C	-6.32487400	-1.46983200	-0.99310400
H	-6.07379200	-0.73383800	-1.76491100
H	-7.29518500	-1.19599500	-0.56733600
C	-0.73557100	-3.89045400	-0.42953900
C	0.36522900	-3.80821800	-1.29991400
C	-0.55138900	-4.26644100	0.91835600
C	0.22657900	-3.45053800	-2.67858900
C	1.68404800	-4.08718300	-0.80172600
C	0.77364200	-4.50173000	1.41386000
C	1.30963500	-3.41025600	-3.50502500
H	-0.75143200	-3.17087500	-3.05307600
C	2.79236400	-4.03926700	-1.70461200
C	1.85965500	-4.39967300	0.54464200
C	2.61064300	-3.72237500	-3.01761000
H	1.18381500	-3.09866200	-4.53557900
H	3.78689900	-4.24510900	-1.31734800
H	2.86241200	-4.58288000	0.92351100
H	3.46227200	-3.67049100	-3.68826100
C	-3.14083900	3.25084800	-0.04387500

C	-2.15822900	3.89917300	0.73197300
C	-3.36049000	3.64516300	-1.38056900
C	-1.89962700	3.56411200	2.10048900
C	-1.37324800	4.95072500	0.15046500
C	-2.55337700	4.68237500	-1.95556000
C	-0.97243300	4.24283500	2.83509100
H	-2.45725600	2.75137100	2.55264100
C	-0.39496900	5.62244600	0.94998200
C	-1.58155300	5.30824300	-1.17889400
C	-0.20441300	5.29122100	2.25612900
H	-0.80188800	3.97123200	3.87326200
H	0.19238200	6.41102600	0.48658700
H	-0.97711400	6.09866700	-1.61875300
H	0.54211800	5.80567600	2.85326600
C	-1.43347900	-4.81229900	3.12782500
H	-2.28061600	-4.95768600	3.79226500
C	-1.64496800	-4.45008000	1.82875300
H	-2.65824500	-4.31310800	1.46690100
C	-0.11266800	-5.00952000	3.62206900
H	0.03757200	-5.28886900	4.66068600
C	0.95405000	-4.85773600	2.78755100
H	1.96795600	-5.00667300	3.14826000
C	-4.55791100	3.46267700	-3.49417700
H	-5.33636700	3.00428600	-4.09645200
C	-3.73154800	4.46906900	-4.06881000
H	-3.88095000	4.76090100	-5.10378300
C	-2.76443500	5.06272500	-3.31759600
H	-2.13144300	5.83936000	-3.73891700
C	-4.38173400	3.06820900	-2.20210600
H	-5.02848200	2.30591100	-1.78323600
N	-1.19454700	-0.56732500	-2.06212600
S	0.03731700	0.03662600	-2.83080400
O	0.15054700	-0.54266300	-4.15557000
O	1.25745800	0.13102200	-2.01133800
C	-0.38606300	1.81864600	-3.12659400
F	-1.58092400	1.92907500	-3.69081600
F	0.52616100	2.37339200	-3.91958000
F	-0.39629900	2.48026100	-1.96490700
C	-0.77794600	-0.44858600	3.91164000
C	-0.14624600	0.97444800	3.84734700
H	-0.51388700	1.54113100	4.71751300
H	-0.55477600	1.48390500	2.97563000
C	1.95283100	2.10139500	2.90264400
C	1.41573600	2.27964300	1.61445600

C	3. 13975700	2. 78629500	3. 23353400
C	2. 07600400	3. 05731800	0. 67421200
H	0. 50775200	1. 77639400	1. 30514100
C	3. 77584500	3. 59205600	2. 30212000
H	3. 55211500	2. 71257200	4. 23453200
C	3. 25670000	3. 71068100	1. 01278300
H	1. 65891300	3. 13513300	-0. 32349700
H	4. 69275300	4. 10565100	2. 56939600
H	3. 78008600	4. 30957700	0. 27456200
C	1. 34318000	1. 16383100	3. 84944600
C	0. 03672600	-1. 48440400	3. 09514500
H	0. 78019800	-1. 97936300	3. 71960900
H	-0. 64901200	-2. 25521800	2. 73320100
N	0. 72289700	-0. 91607100	1. 95183000
C	2. 00805700	-1. 06156600	1. 62764000
N	2. 35435400	-0. 65044400	0. 39730300
C	3. 66532600	-0. 37886400	-0. 06514800
C	4. 52381900	0. 45602900	0. 64472900
C	4. 04615500	-0. 88624500	-1. 29883200
C	5. 77888500	0. 74503200	0. 12838600
C	5. 31154700	-0. 59680700	-1. 79945200
H	3. 35140300	-1. 49726400	-1. 86181800
C	6. 18868400	0. 21399800	-1. 09275100
H	7. 17334400	0. 43480300	-1. 48663900
C	5. 71930700	-1. 23621400	-3. 09920400
C	6. 66857800	1. 71099500	0. 86018800
F	4. 78141000	-1. 08276400	-4. 04372000
F	6. 86772600	-0. 73127100	-3. 57592800
F	5. 90241300	-2. 56453700	-2. 94642100
F	6. 47326800	1. 66947100	2. 18946600
F	7. 96880500	1. 46840400	0. 63424700
F	6. 43785400	2. 98422400	0. 47589600
S	3. 17329200	-1. 68268300	2. 74377300
H	4. 20861300	0. 87954100	1. 58979400
H	1. 62765100	-0. 44417100	-0. 29840500
H	0. 11838700	-0. 42628000	1. 27438900
C	2. 16781300	0. 42739100	4. 70830200
H	1. 70836200	-0. 07608100	5. 55410100
H	2. 53461600	-0. 53335800	3. 92297300
H	3. 17278400	0. 80184600	4. 90099300
C	-2. 19840900	-0. 30527100	3. 33239000
H	-2. 78694500	0. 40937000	3. 92068600
H	-2. 71870900	-1. 26925400	3. 35182600
H	-2. 17522100	0. 04436900	2. 29874600

C	-0.91565000	-0.99762900	5.34023200
H	-1.39997000	-1.98047300	5.30920500
H	-1.53812400	-0.33757900	5.95429300
H	0.04515700	-1.13100900	5.84537000

TS-EF-1R-2-蠅B97X-D

l imaginary frequencies

H = -5197.527958

G = -5197.706877

E(M06-2X-DCM) = -5199.574272

O	-2.70865400	0.35295900	-1.20541200
O	-2.41636500	-1.01789800	0.93888200
P	-1.61700600	-0.04600000	-0.08937500
O	-1.15059700	1.09461900	0.75260300
C	-6.23066200	2.21268600	-0.00021900
C	-6.12556700	0.82933800	-0.00571900
C	-4.96011500	0.20542500	-0.45571300
C	-3.93845900	2.38522800	-0.80798600
C	-5.14509300	2.97645800	-0.41944600
C	-2.86336400	-2.24138600	0.46937300
C	-4.03475800	-2.31014200	-0.27062900
C	-4.36756400	-3.51297100	-0.89900700
C	-3.62479800	-4.66082800	-0.66940500
C	-2.52525200	-4.59572800	0.18052900
C	-2.10192800	-3.38509400	0.73891000
H	-5.21140300	4.06041500	-0.41990000
H	-1.94610300	-5.49067400	0.38667800
C	-5.14872800	-1.29962500	-0.49807000
C	-6.25742800	-1.46237800	0.58595100
H	-5.77993500	-1.47495700	1.57245500
H	-6.81754900	-2.39512100	0.47371800
H	-6.46205600	-3.77578900	-1.38892300
H	-5.39790300	-3.77235200	-2.79372400
C	-3.87538100	0.98646200	-0.81713900
H	-7.14274000	2.69819500	0.33519800
H	-3.89149400	-5.59967500	-1.14607500
C	-7.12887500	-0.20245400	0.44912400
H	-7.62309500	0.07539900	1.38527700
H	-7.91704800	-0.34219000	-0.30216600
C	-5.55692700	-3.31970300	-1.81010200
C	-5.67532900	-1.78545100	-1.87724800
H	-5.01126800	-1.39780200	-2.65714000
H	-6.69040100	-1.43397600	-2.08568500
C	-0.88053500	-3.35014400	1.59620700

C	0.35495200	-3.77636900	1.06461600
C	-0.97868700	-3.00390400	2.96237000
C	0.52480800	-4.12348800	-0.31607100
C	1.50121100	-3.88332500	1.92277300
C	0.18222200	-3.09143700	3.80241900
C	1.70386500	-4.62869500	-0.77617400
H	-0.29342400	-3.95504100	-1.00413600
C	2.73005500	-4.39185000	1.39366200
C	1.39298500	-3.52216000	3.26328700
C	2.82224000	-4.78474900	0.09377800
H	1.81168800	-4.86671900	-1.82895900
H	3.58589400	-4.46339900	2.05937800
H	2.26593300	-3.59777300	3.90721200
H	3.75868500	-5.16278100	-0.30273700
C	-2.75782700	3.21886900	-1.17081200
C	-2.17272400	4.05766800	-0.19917100
C	-2.23176900	3.16685800	-2.47617100
C	-2.64700800	4.13801600	1.15094500
C	-1.04086000	4.86389100	-0.55292200
C	-1.07893100	3.95361800	-2.80602000
C	-2.08132500	4.99207900	2.05097500
H	-3.46703000	3.49984300	1.45895800
C	-0.45404300	5.72136300	0.42984400
C	-0.51916000	4.78780700	-1.84223200
C	-0.96631800	5.80072000	1.68924700
H	-2.47052400	5.04198400	3.06433700
H	0.41186100	6.31264600	0.14316500
H	0.35487100	5.38350800	-2.09644400
H	-0.52259800	6.46768700	2.42308100
C	-2.27329000	-2.29012700	4.90448000
H	-3.22064800	-1.98779600	5.34109600
C	-2.20750200	-2.59545200	3.57619600
H	-3.10498700	-2.54173800	2.97102000
C	-1.11665600	-2.37691300	5.73119300
H	-1.19008200	-2.13682000	6.78778300
C	0.07195300	-2.76709600	5.19189000
H	0.96520000	-2.84001700	5.80687000
C	-2.25301800	2.30820800	-4.75282800
H	-2.69869000	1.67650700	-5.51497700
C	-1.08673300	3.06233200	-5.06429900
H	-0.65290600	2.99365600	-6.05712700
C	-0.52482400	3.86603700	-4.12130600
H	0.35940000	4.45647400	-4.34783400
C	-2.80729400	2.36232900	-3.51070300

H	-3.69729200	1.78260600	-3.29453700
N	-0.50904500	-0.93557600	-0.83759100
S	-0.03507400	-0.76974200	-2.34809200
O	1.16078300	-1.57700600	-2.54149700
O	-0.04385200	0.60480900	-2.83575000
C	-1.31771700	-1.66286900	-3.36919700
F	-1.70857700	-2.78104300	-2.75361200
F	-0.77594100	-1.98693900	-4.53922700
F	-2.39280700	-0.91343700	-3.59694100
C	-0.18127300	1.75703000	4.10002600
C	0.38701700	2.85803700	3.15631000
H	0.17798000	3.83579500	3.61681200
H	-0.20094900	2.85591200	2.23767400
C	2.24514200	3.19273700	1.42020200
C	1.49173800	2.71870800	0.33202900
C	3.44612400	3.88035200	1.15434200
C	1.96236900	2.85001800	-0.96851100
H	0.55281900	2.19835400	0.48316900
C	3.88658600	4.05548000	-0.14813100
H	4.02241000	4.30716900	1.96886600
C	3.16008500	3.51552100	-1.20965900
H	1.38735400	2.41868200	-1.78285100
H	4.81519600	4.58300600	-0.33642100
H	3.53485000	3.61077400	-2.22368200
C	1.84648700	2.89600600	2.80179300
C	0.44018200	0.36222300	3.82142500
H	1.29664400	0.17221300	4.46819300
H	-0.31146900	-0.39895900	4.04564400
N	0.87028700	0.17813700	2.44695900
C	2.06165500	-0.23748700	2.02178000
N	2.15655200	-0.56630400	0.71926000
C	3.35535800	-0.60840000	-0.04021300
C	4.28207300	0.42954700	0.01809900
C	3.55729500	-1.67520700	-0.90343000
C	5.43066400	0.36582700	-0.75896600
C	4.70523200	-1.71954100	-1.68645100
H	2.80738900	-2.44950900	-0.97579300
C	5.65387200	-0.70893700	-1.61464600
H	6.55151300	-0.75228700	-2.22009900
C	4.94997400	-2.92020200	-2.55969800
C	6.41513700	1.50154400	-0.73125600
F	3.81557700	-3.41386100	-3.07046600
F	5.77086700	-2.63542200	-3.58376100
F	5.53244400	-3.91916600	-1.86130600

F	6.39714200	2.15956700	0.44065900
F	7.67265800	1.07594000	-0.93418500
F	6.15677500	2.41162500	-1.69308200
S	3.42942100	-0.30018300	3.07946600
H	4.11051900	1.27942400	0.66584200
H	1.28802600	-0.77612700	0.21079900
H	0.14268800	0.37312800	1.74493000
C	2.84083400	2.61523500	3.74062300
H	2.58328200	2.64064700	4.79504800
H	3.05372900	1.32881800	3.52066900
H	3.86097900	2.92541200	3.51607400
C	-1.70017300	1.70385400	3.84597000
H	-2.15376100	2.68303700	4.03685000
H	-2.16750100	0.97388600	4.51656600
H	-1.92283700	1.42143900	2.81425800
C	0.01707200	2.06265900	5.59369600
H	-0.45344700	1.27593400	6.19483600
H	-0.45753800	3.01326900	5.86041800
H	1.06724900	2.10907700	5.89418700

INT-7

0 imaginary frequencies

H = -4967.768516

G = -4967.955012

E(M06-2X-DCM) = -4968.556560

O	1.50016900	-2.12966700	-0.26982700
O	3.02673700	-0.09703000	0.21522400
P	1.46821400	-0.49923300	-0.06550900
O	0.68748000	-0.11093800	1.15528700
C	2.90230600	-4.47631000	2.90739900
C	3.78719500	-3.90281300	2.00075700
C	3.31214900	-3.17630000	0.89828200
C	1.02089700	-3.52811300	1.66014600
C	1.53222300	-4.30879800	2.71164700
C	3.98672400	-0.32254300	-0.77546500
C	4.52161300	-1.60065600	-0.93334400
C	5.34560000	-1.86484000	-2.03883300
C	5.72934700	-0.84186400	-2.89876100
C	5.28968600	0.45646900	-2.64290800
C	4.40349200	0.74664700	-1.59197500
H	0.82859200	-4.77263400	3.39677400
H	5.61424400	1.27308900	-3.28089000
C	4.46833900	-2.83279200	-0.03412500
C	5.65395400	-2.82253900	0.99107800

H	5. 67576400	-1. 84796400	1. 49245200
H	6. 62483500	-2. 97059200	0. 50852800
H	6. 73366100	-3. 51913200	-1. 81654200
H	5. 57033100	-3. 74688600	-3. 11759400
C	1. 94374800	-2. 94174300	0. 77089800
H	3. 26709400	-5. 05120200	3. 75494600
H	6. 37242400	-1. 04308200	-3. 75189300
C	5. 29980800	-3. 92434500	2. 01215800
H	5. 71569800	-3. 73010600	3. 00751300
H	5. 68606600	-4. 90340300	1. 69534600
C	5. 68959500	-3. 33724400	-2. 10801000
C	4. 70482000	-3. 95966800	-1. 09424300
H	3. 75264200	-4. 18046600	-1. 59003500
H	5. 07129100	-4. 88770400	-0. 64401500
C	3. 99518100	2. 16767800	-1. 36177100
C	3. 24592200	2. 85889500	-2. 34524900
C	4. 46062600	2. 85177600	-0. 20998400
C	2. 71990400	2. 21764000	-3. 51268500
C	2. 97484800	4. 26915400	-2. 17633200
C	4. 16426300	4. 25729600	-0. 04654400
C	2. 01221800	2. 91958000	-4. 45180200
H	2. 85134000	1. 14909400	-3. 62720000
C	2. 23878600	4. 96579800	-3. 18532000
C	3. 43604000	4. 92651900	-1. 03352100
C	1. 77606400	4. 31461300	-4. 29585600
H	1. 60190200	2. 40051900	-5. 31300100
H	2. 05132400	6. 02776800	-3. 04370900
H	3. 22536200	5. 98696900	-0. 90988600
H	1. 21219700	4. 85267400	-5. 05315500
C	-0. 46202200	-3. 38539100	1. 52550600
C	-1. 20241500	-2. 74935600	2. 55368000
C	-1. 13566500	-3. 97402400	0. 42671800
C	-0. 58339400	-2. 11991300	3. 68255500
C	-2. 64616400	-2. 72180700	2. 48426200
C	-2. 57819500	-3. 90974800	0. 35358200
C	-1. 32897000	-1. 55649900	4. 68679500
H	0. 49818400	-2. 09122100	3. 73430500
C	-3. 38712300	-2. 11590900	3. 54786600
C	-3. 29403100	-3. 29528000	1. 38604700
C	-2. 75254100	-1. 55895600	4. 62631400
H	-0. 82904200	-1. 10720000	5. 54158800
H	-4. 47285900	-2. 12003000	3. 48431200
H	-4. 38006300	-3. 26456700	1. 33222000
H	-3. 32987700	-1. 12392500	5. 43854400

C	5. 69293400	2. 91612000	1. 90419700
H	6. 29501900	2. 41056300	2. 65482100
C	5. 25194700	2. 22401200	0. 80593900
H	5. 51332400	1. 17810800	0. 69390100
C	5. 38250200	4. 29652500	2. 06746300
H	5. 74606000	4. 83232900	2. 94053000
C	4. 64290800	4. 94377400	1. 11383900
H	4. 41150400	6. 00192600	1. 21424700
C	-1. 13332500	-5. 22814400	-1. 66971300
H	-0. 58673500	-5. 74629300	-2. 45288300
C	-2. 55142700	-5. 13482100	-1. 75052200
H	-3. 07259000	-5. 57458500	-2. 59638300
C	-3. 25194500	-4. 49713100	-0. 76345900
H	-4. 33403900	-4. 41667000	-0. 81185200
C	-0. 45199200	-4. 67090300	-0. 62006100
H	0. 62711800	-4. 75679600	-0. 57513900
C	0. 84693800	2. 54418200	3. 77440900
C	1. 27791000	3. 33761600	2. 50340800
H	2. 31303800	3. 66511300	2. 65388800
H	1. 29934400	2. 64609100	1. 65131800
C	0. 42170400	4. 52774900	2. 15862600
C	-0. 65138700	2. 15275200	3. 72189500
H	-1. 24547800	3. 06455700	3. 82959300
H	-0. 87548300	1. 49219900	4. 57120200
N	-1. 07383600	1. 49240500	2. 47539600
C	-2. 30397100	1. 48321200	1. 99011300
N	-2. 56845900	0. 97842200	0. 77968700
C	-3. 84585000	0. 95658200	0. 14257700
C	-4. 56332100	2. 13709500	-0. 06912600
C	-4. 33958600	-0. 26192900	-0. 32546400
C	-5. 81017800	2. 08297000	-0. 69157600
C	-5. 58241100	-0. 29806100	-0. 95873300
H	-3. 75148800	-1. 16325300	-0. 19787100
C	-6. 32887600	0. 86609600	-1. 13438200
H	-7. 29853900	0. 82750100	-1. 61524000
C	-6. 11272000	-1. 63056900	-1. 42610200
C	-6. 57077300	3. 35836700	-0. 95364700
F	-7. 30539800	-1. 51664700	-2. 04293500
F	-6. 28289500	-2. 48335400	-0. 38097700
F	-5. 26226800	-2. 23186100	-2. 27967300
F	-7. 90494700	3. 15475600	-0. 91197100
F	-6. 28391000	3. 86736200	-2. 16995300
F	-6. 27230000	4. 31039200	-0. 04237000
S	-3. 68372100	2. 14145500	2. 90975000

H	-4.15045300	3.09359000	0.23142100
H	-1.82323900	0.50415600	0.23272500
H	-0.36281600	0.93429900	1.95141500
C	0.79764400	5.80308900	2.27354200
H	1.78732100	6.07373600	2.63577300
H	-3.10543900	1.97614300	4.11361100
H	0.14037900	6.62259600	1.99428400
N	1.10833700	0.11321800	-1.51009400
S	-0.33720400	0.09616600	-2.15346400
O	-0.64987900	1.33320600	-2.86982000
O	-1.39080000	-0.44312400	-1.24103800
C	-0.20273200	-1.20348900	-3.48776600
F	0.72497800	-0.83676400	-4.38250400
F	-1.37850900	-1.32787700	-4.11356300
F	0.14141900	-2.38540300	-2.96924800
C	1.74592400	1.30256100	3.92742100
H	1.50350200	0.75942200	4.85009100
H	1.65218100	0.61591900	3.08258600
H	2.79571400	1.61144000	3.98805400
C	1.00522100	3.42942300	5.02779000
H	0.66094700	2.90760600	5.92980000
H	2.06104000	3.68072900	5.17613200
H	0.44829200	4.36798200	4.93594300
H	-0.57524900	4.31471800	1.76891900

INT-7'

0 imaginary frequencies

H = -4967.786356

G = -4967.970063

E(M06-2X-DCM) = -4968.564088

C	0.75144900	-3.06305400	-4.21769600
C	0.47246000	-1.79296600	-5.07908200
H	1.34768100	-1.63107100	-5.72241000
H	-0.36741500	-2.02708800	-5.75087400
C	0.15731000	-0.49804700	-4.37644400
C	-0.50816300	-3.56838200	-3.47320200
H	-0.29368300	-4.56150200	-3.05079000
H	-1.33198100	-3.70198400	-4.17939000
N	-0.97535000	-2.68427800	-2.41330600
C	-2.21512000	-2.75619300	-1.85521400
N	-2.32409600	-1.91655500	-0.76351400
C	-3.38105300	-1.64188200	0.11004800
C	-4.74210600	-1.82586600	-0.18289100
C	-3.02665600	-1.08508500	1.35161200

C	-5.70425100	-1.46926900	0.76183600
C	-4.00327200	-0.73619300	2.27972700
H	-1.97950300	-0.92192100	1.58515400
C	-5.35577600	-0.93113300	2.00083000
H	-6.11645800	-0.67253100	2.72724200
C	-3.59241700	-0.06598500	3.55986500
C	-7.16237000	-1.57328100	0.39811800
F	-4.49146100	-0.24518100	4.54756000
F	-3.45626400	1.28211300	3.39857500
F	-2.39537800	-0.51144000	4.01248300
F	-7.61501500	-0.41082000	-0.14447500
F	-7.93479700	-1.81728000	1.48054500
F	-7.40137600	-2.54409500	-0.50275600
S	-3.42904000	-3.76628500	-2.44283400
C	1.14411100	-4.19316200	-5.19429300
H	2.03430700	-3.91622300	-5.77048800
H	1.36988100	-5.12016200	-4.65464300
H	0.33639600	-4.40619100	-5.90494800
C	1.92882600	-2.81927100	-3.25526800
H	2.14921400	-3.71858600	-2.66995100
H	2.83167700	-2.55423600	-3.81906200
H	1.74191300	-2.00351700	-2.54964900
H	-5.03362800	-2.24694200	-1.13423700
C	0.90510100	0.60902100	-4.46810000
H	-1.45492900	-1.45380500	-0.49755400
H	1.83211600	0.62848700	-5.03846200
H	0.59061600	1.55341100	-4.03263800
H	-0.26190500	-2.19405000	-1.88204700
H	1.63253600	0.73170000	-2.21744700
O	-0.07268800	1.44410800	0.52754600
O	2.19514600	0.32149300	1.11605300
P	1.04267200	0.41260900	-0.00303900
O	0.36128300	-0.84016400	-0.41455200
C	0.96859500	5.40143400	1.42555700
C	1.29694300	4.37359900	2.30237900
C	0.85610900	3.06261800	2.06375400
C	-0.18716100	3.80287700	-0.02386400
C	0.19415700	5.11594300	0.30190400
C	1.84123900	-0.17493400	2.39746100
C	1.26895800	0.69874700	3.31830800
C	0.79561600	0.17540600	4.53395600
C	0.97567700	-1.16557700	4.85194600
C	1.62995500	-1.99737900	3.94532900
C	2.06275500	-1.53318700	2.69225400

H	-0.10948600	5.91811100	-0.36358800
H	1.79501300	-3.04272700	4.18826200
C	1.09732100	2.21530600	3.30949400
C	2.35046600	2.94377000	3.89845800
H	2.48291300	2.74615700	4.96660800
H	3.24505000	2.58743900	3.37515000
H	-0.85399900	0.88379400	5.75798100
H	0.71198800	1.57806200	6.18229100
C	0.21099400	2.78536200	0.86335500
H	1.29554500	6.42018400	1.61681800
H	0.60965700	-1.56527400	5.79388200
C	2.11533200	4.43609300	3.57395500
H	1.56624400	4.94181300	4.38000800
H	3.05168100	4.98814200	3.43620500
C	0.09180400	1.24239500	5.33966200
C	-0.11101700	2.36135100	4.29905300
H	-0.16674300	3.36148300	4.73836100
H	-1.04398400	2.18237900	3.75506300
C	2.75101400	-2.49340900	1.77100600
C	4.15996500	-2.44320600	1.63880700
C	2.00886700	-3.51715300	1.13465400
C	4.97229300	-1.49131400	2.33415800
C	4.83204500	-3.41269700	0.80357600
C	2.69783400	-4.49512100	0.32217100
C	6.33559800	-1.47795700	2.19308100
H	4.49276100	-0.77180500	2.98877800
C	6.25449000	-3.35334100	0.67030500
C	4.08368100	-4.40658000	0.16685500
C	6.98925100	-2.41419200	1.34255300
H	6.92720100	-0.74568100	2.73590100
H	6.74146300	-4.08383600	0.02863500
H	4.59606800	-5.14188000	-0.45039400
H	8.07037900	-2.38434200	1.23892900
C	-1.01860200	3.55221700	-1.24250700
C	-2.34507300	3.06823300	-1.10260100
C	-0.51245800	3.88237500	-2.52593900
C	-2.94676700	2.78652500	0.16545900
C	-3.16012800	2.86926600	-2.28057500
C	-1.35474700	3.71236800	-3.69011000
C	-4.22767200	2.30876200	0.25921100
H	-2.37947000	2.96168900	1.07217300
C	-4.48548200	2.34985500	-2.13961600
C	-2.64505800	3.19887200	-3.53665600
C	-5.00755500	2.06715400	-0.90691000

H	-4.64773100	2.10241300	1.23778500
H	-5.06991400	2.18422100	-3.04144300
H	-3.26792600	3.05907300	-4.41782300
H	-6.00504900	1.64924900	-0.80895500
C	-0.09753100	-4.66041200	0.64808200
H	-1.17601500	-4.73043400	0.75613900
C	0.58723400	-3.64370000	1.26106100
H	0.04877600	-2.91572800	1.85666900
C	0.58853800	-5.62731200	-0.14210900
H	0.02718000	-6.42791700	-0.61531000
C	1.94572300	-5.54158200	-0.29995200
H	2.48277600	-6.27437100	-0.89787300
C	1.26842900	4.69022200	-3.99662100
H	2.28725000	5.04365800	-4.12555100
C	0.42430600	4.54721700	-5.13358600
H	0.79797000	4.80987400	-6.11936000
C	-0.84773800	4.06568000	-4.98002500
H	-1.50044800	3.93646400	-5.84004700
C	0.81804200	4.37009700	-2.74153000
H	1.48334300	4.47894800	-1.89314700
N	1.92981000	1.05652700	-1.28852700
S	3.34142300	1.97618200	-1.35619100
C	4.71232300	0.76383600	-0.86856500
O	3.32005000	3.00252000	-0.32529900
O	3.54678200	2.26010400	-2.76993700
F	4.34458000	-0.48438800	-1.15224000
F	5.79378300	1.08423500	-1.57615500
F	4.97354900	0.88693300	0.42536500
H	-0.77309600	-0.46212300	-3.81204700

TS-EF-2S

l imaginary frequencies

H = -4967.753505

G = -4967.933851

E(M06-2X-DCM) = -4968.529806

O	3.10693300	0.50955400	-0.69800300
O	1.24438400	2.17331200	0.00681100
P	1.52508100	0.58638400	-0.28374200
O	0.73699800	0.05347300	-1.44095300
N	1.43494900	-0.14463100	1.15817400
S	0.10103500	-0.33700500	1.97807900
C	0.32389700	0.76696500	3.46832700
F	-0.76030200	0.68435900	4.24544400
F	1.39329200	0.38109200	4.18024300

F	0.49501400	2.03269200	3.08423700
O	-0.01443000	-1.69685300	2.53144800
O	-1.11817400	0.21848700	1.32365000
C	1.65402400	4.70787800	-3.30251600
C	2.75861200	4.35660500	-2.53339700
C	2.60288900	3.57298900	-1.38088400
C	0.20346400	3.42213500	-1.80406900
C	0.38962100	4.26575200	-2.91358500
C	4.08857200	0.96953100	0.18312300
C	4.34372900	2.33882600	0.27505900
C	5.21042500	2.80649000	1.27613900
C	5.89867200	1.91821900	2.09466000
C	5.72765700	0.54892900	1.89821200
C	4.82071200	0.04260400	0.95212600
H	-0.48409900	4.55668200	-3.48921200
H	6.29240800	-0.15838500	2.49836200
C	3.91688900	3.50594800	-0.61348600
C	4.93210300	3.72017000	-1.78782600
H	5.90300300	4.08617800	-1.43968100
H	5.09730100	2.75929700	-2.28894400
H	5.16044900	4.72722700	2.30789300
H	6.18224700	4.70298300	0.87477100
C	1.34681000	3.06127400	-1.06634100
H	1.76691900	5.32326900	-4.19159600
H	6.57256000	2.28009300	2.86706900
C	4.21777800	4.69303600	-2.75191600
H	4.42845500	5.74016500	-2.49265900
H	4.52891400	4.55943400	-3.79435000
C	5.24148700	4.31915500	1.29393300
C	4.03560600	4.68903800	0.40488100
H	4.14107400	5.65837300	-0.09224200
H	3.12390000	4.72178800	1.01224900
C	4.74535400	-1.44262300	0.77041800
C	5.29142200	-2.03082800	-0.39894200
C	4.26117900	-2.26408100	1.81785900
C	5.82373900	-1.26033400	-1.48280900
C	5.35619700	-3.47141300	-0.51120500
C	4.34566100	-3.70306900	1.69888000
C	6.35318000	-1.85893100	-2.59633200
H	5.80911900	-0.17900600	-1.41220600
C	5.91628800	-4.05679000	-1.69060600
C	4.89029700	-4.26616500	0.54111500
C	6.39813500	-3.27769200	-2.70813200
H	6.74831700	-1.24643500	-3.40227400

H	5.95826400	-5.14192800	-1.75534700
H	4.96565700	-5.34945900	0.46157200
H	6.82403200	-3.73548700	-3.59693800
C	-1.18125100	2.98450100	-1.44667400
C	-1.77674700	3.43245000	-0.24098800
C	-1.92826300	2.19755600	-2.35882300
C	-1.08826900	4.24756400	0.71353300
C	-3.14783500	3.08066200	0.05093600
C	-3.31678100	1.90502600	-2.08123200
C	-1.68694800	4.64050900	1.88159600
H	-0.07156000	4.55779500	0.50306800
C	-3.73285400	3.50008100	1.28677200
C	-3.88536600	2.34950800	-0.88456900
C	-3.02316700	4.25270800	2.18232200
H	-1.13611900	5.25350800	2.59000300
H	-4.75042900	3.18959300	1.50722000
H	-4.92720100	2.11771900	-0.67378500
H	-3.47544700	4.55938800	3.12146200
C	3.21002400	-2.54755400	4.00424700
H	2.73612800	-2.11241200	4.87890100
C	3.66774200	-1.72920400	3.00583800
H	3.54638500	-0.65744500	3.09036800
C	3.32041400	-3.96273700	3.89388200
H	2.95704000	-4.59491000	4.69969800
C	3.86885500	-4.52130900	2.77118000
H	3.95216800	-5.60131300	2.67090700
C	-2.12431700	0.92218300	-4.43642400
H	-1.66954300	0.52106700	-5.33868900
C	-3.50481800	0.67984700	-4.18046000
H	-4.09446300	0.11319000	-4.89645800
C	-4.07986100	1.15412900	-3.03183900
H	-5.12813300	0.96160500	-2.81560700
C	-1.36485600	1.65211900	-3.55875200
H	-0.31120200	1.80776000	-3.75647200
C	1.11624200	-3.55579100	-2.34254500
C	1.36094200	-3.59956500	-0.79808700
H	2.19101300	-4.30044900	-0.61190500
H	1.72430700	-2.62322900	-0.46913400
C	0.24289000	-3.98958300	0.10813600
C	-0.30017700	-2.98128000	-2.67299900
H	-0.99498200	-3.78614200	-2.91077000
H	-0.22102600	-2.33872700	-3.55791100
N	-0.92002500	-2.17454400	-1.61570000
C	-2.18790200	-2.31215300	-1.18622200

N	-2.69031700	-1.30441600	-0.44198800
C	-4.02005000	-1.15193500	0.02079000
C	-5.11129000	-1.39611100	-0.81481300
C	-4.22574400	-0.64466000	1.31063700
C	-6.40531400	-1.15430800	-0.35271100
C	-5.52501200	-0.40786100	1.75468200
H	-3.37328200	-0.42544500	1.94324600
C	-6.62465900	-0.66560200	0.93276300
H	-7.63229700	-0.48395700	1.28724500
C	-5.76438400	0.19124300	3.11633400
C	-7.55150900	-1.33271800	-1.31193300
F	-6.03971200	1.51790100	3.02750400
F	-4.70187300	0.05755000	3.93015400
F	-6.82707900	-0.37958100	3.72656200
F	-7.42858200	-2.46481400	-2.03657000
F	-7.60347400	-0.30661200	-2.20056000
F	-8.74333600	-1.37334100	-0.68355500
S	-3.05212000	-3.80146500	-1.43242100
H	-4.95622800	-1.74027200	-1.82938400
H	-2.02461800	-0.61957500	-0.05676700
H	-0.43561400	-1.26976300	-1.44894700
C	1.23163200	-4.94963200	-2.99415400
H	2.23332000	-5.36604400	-2.83991300
H	0.50027800	-5.66525600	-2.60485700
H	1.06966300	-4.87676500	-4.07648600
C	2.20823700	-2.65088100	-2.95188400
H	2.11746400	-1.62173500	-2.59426700
H	3.20792600	-3.01913600	-2.69938500
H	2.12290500	-2.64351000	-4.04569900
C	-0.63352500	-5.06378200	-0.02752400
H	-0.37777700	-5.87397000	-0.70954200
H	-1.66038900	-4.54402300	-0.66469700
H	-1.15893100	-5.37822900	0.87537900
H	0.10692200	-3.34845700	0.98195800

TS-EF-2S-1

l imaginary frequencies

H = -4967.750498

G = -4967.929329

E(M06-2X-DCM) = -4968.524649

O	2.63186200	0.61956000	0.51169300
O	0.44245300	1.98686700	0.34540800
O	0.23245200	-0.46448300	0.75658500
C	3.53467600	1.81932200	4.41683100

C	3. 32444800	2. 76509300	3. 41899400
C	3. 06117500	2. 37495600	2. 09528700
C	3. 16381300	0. 03207500	2. 79501700
C	3. 46947700	0. 46369100	4. 09480700
C	0. 85736200	3. 12774400	-0. 34706600
C	2. 07364000	3. 72452700	-0. 03328700
C	2. 58393100	4. 70749800	-0. 89488200
C	1. 81448300	5. 19729600	-1. 94455000
C	0. 52280300	4. 70083200	-2. 13256300
C	0. 02235400	3. 64490000	-1. 35624900
H	3. 64067700	-0. 28598100	4. 86198500
H	-0. 10697800	5. 11166100	-2. 91643300
C	2. 98494000	3. 60071100	1. 18651700
C	2. 59288800	4. 69459400	2. 24328400
H	1. 50764300	4. 66117100	2. 39417800
H	2. 85119200	5. 70444400	1. 91184000
H	4. 06351000	6. 06910200	-0. 06183400
H	4. 67998700	5. 05638400	-1. 36396300
C	2. 94718200	1. 01628300	1. 81187000
H	3. 74119100	2. 12828200	5. 43837400
H	2. 20437100	5. 96444000	-2. 60862600
C	3. 30580600	4. 27136400	3. 54213900
H	2. 78743700	4. 61547100	4. 44422500
H	4. 32654000	4. 67672200	3. 58910500
C	4. 00319200	5. 06414300	-0. 50235200
C	4. 35621200	3. 96865800	0. 53310400
H	4. 74665000	3. 08458400	0. 01660000
H	5. 10014800	4. 29030400	1. 26940100
C	-1. 36974200	3. 12932600	-1. 55603200
C	-1. 72217300	2. 42912900	-2. 73525200
C	-2. 34848200	3. 37996400	-0. 56013600
C	-0. 78090500	2. 14617300	-3. 77712800
C	-3. 07795200	1. 95201000	-2. 90613500
C	-3. 69398500	2. 88287300	-0. 73670500
C	-1. 15004300	1. 45824900	-4. 90397300
H	0. 24564800	2. 47239900	-3. 66003200
C	-3. 42220700	1. 24430900	-4. 10096400
C	-4. 02181700	2. 18187000	-1. 90125300
C	-2. 48944800	1. 00499100	-5. 07451000
H	-0. 40655500	1. 24552100	-5. 66637500
H	-4. 44873600	0. 90390300	-4. 21898300
H	-5. 03644400	1. 80803600	-2. 02384200
H	-2. 76600100	0. 46866600	-5. 97866700
C	3. 09652800	-1. 43418200	2. 49592300

C	2. 01520200	-2. 20804000	2. 98134000
C	4. 14871400	-2. 05058800	1. 77607300
C	0. 91801900	-1. 64063200	3. 70778100
C	1. 98891800	-3. 63229000	2. 73221800
C	4. 10317100	-3. 47257600	1. 52148900
C	-0. 11191100	-2. 41747000	4. 17114600
H	0. 90348900	-0. 57054600	3. 87752600
C	0. 89648700	-4. 40889600	3. 23517000
C	3. 02678900	-4. 22278900	2. 00514200
C	-0. 12304400	-3. 82319400	3. 93649500
H	-0. 93514900	-1. 96004400	4. 71102900
H	0. 90170700	-5. 48150200	3. 05309800
H	3. 00426700	-5. 29596800	1. 82368300
H	-0. 94440000	-4. 42391700	4. 31822900
C	-3. 04024600	4. 35284700	1. 57416900
H	-2. 80241100	4. 93085400	2. 46328600
C	-2. 07422600	4. 13206600	0. 62753800
H	-1. 08060900	4. 54157400	0. 76927300
C	-4. 35528100	3. 83386100	1. 40732000
H	-5. 10559800	4. 01120800	2. 17323000
C	-4. 67012400	3. 12192500	0. 28162000
H	-5. 66793700	2. 71563500	0. 14053400
C	6. 29139700	-1. 95115500	0. 60579800
H	7. 14265000	-1. 37578700	0. 25235000
C	6. 23345100	-3. 34941800	0. 34380300
H	7. 03893900	-3. 82752900	-0. 20703400
C	5. 16984700	-4. 08515000	0. 79207600
H	5. 11909100	-5. 15605400	0. 60824400
C	5. 28714500	-1. 32628900	1. 29755000
H	5. 34808200	-0. 26124700	1. 48982400
C	0. 49446800	-3. 85814400	-3. 44434700
C	1. 19952600	-4. 01812600	-2. 05389700
H	1. 73099400	-4. 98045200	-2. 07857200
H	1. 95629000	-3. 23726800	-1. 95457700
C	0. 32873800	-3. 99088400	-0. 83677900
C	-0. 43723400	-2. 59170600	-3. 46082500
H	-1. 37398400	-2. 83119700	-3. 96643600
H	0. 06280000	-1. 78647800	-4. 00287300
N	-0. 76334500	-1. 99869900	-2. 15361400
C	-1. 93324800	-2. 06911000	-1. 49805400
N	-2. 08827400	-1. 23165900	-0. 45456600
C	-3. 21466700	-1. 07734100	0. 38433500
C	-4. 51408800	-0. 99162000	-0. 12089200
C	-2. 98301700	-0. 90996400	1. 75414300

C	-5.57734800	-0.76147100	0.75126100
C	-4.05880400	-0.68616800	2.61228300
H	-1.96630900	-0.94754700	2.13248600
C	-5.36254800	-0.61269800	2.12125500
H	-6.19345700	-0.43020800	2.79092600
C	-3.79858300	-0.58005400	4.09237500
C	-6.95511600	-0.58858900	0.16957400
F	-2.67135600	0.11634300	4.35505000
F	-3.63436500	-1.80472400	4.65407900
F	-4.81396700	0.02061500	4.74603700
F	-7.21978900	-1.51649800	-0.77388900
F	-7.08708100	0.62286400	-0.43632400
F	-7.92009500	-0.66666500	1.10685000
S	-3.03698500	-3.37502000	-1.82762500
H	-4.69283800	-1.07560500	-1.18530800
H	-1.22190300	-0.78503500	-0.08491200
H	-0.11957200	-1.22435200	-1.89389900
C	-0.30733700	-5.11766300	-3.83481600
H	0.32561200	-6.01221200	-3.79487700
H	-1.18344500	-5.28099700	-3.20421000
H	-0.67035700	-5.02003300	-4.86466500
C	1.60616900	-3.65999600	-4.49696700
H	2.20905400	-2.77247000	-4.28428500
H	2.26525000	-4.53545700	-4.53510600
H	1.16873000	-3.53324500	-5.49440400
C	-0.69770700	-4.87877800	-0.54837400
H	-0.73177400	-5.83353300	-1.07257000
H	-1.77236800	-4.29020700	-1.16335400
H	-1.07019200	-4.89548500	0.47574900
H	0.52194300	-3.19787400	-0.11574100
N	1.18043700	0.13910300	-1.55814900
S	2.25937300	0.47712400	-2.69658700
O	1.83662800	-0.22803900	-3.91838300
O	2.66889600	1.88273100	-2.79047500
C	3.84481900	-0.42747900	-2.20502100
F	4.50073000	-0.77717100	-3.31763700
F	4.63864600	0.34874900	-1.46601700
F	3.56280500	-1.54587400	-1.51236800
P	1.08574700	0.52108200	0.01274100

TS-EF-2R

l imaginary frequencies

H = -4967.751444

G = -4967.932684

E(M06-2X-DCM) = -4968.525651

O	0.24693300	-2.29713500	-0.02968200
O	2.56625800	-1.16669300	-0.15824400
P	0.98062600	-0.84874200	0.10696300
O	0.39550200	0.04725500	-0.94119800
N	0.89321100	-0.45142200	1.67323300
S	1.50861200	0.83850200	2.32930700
C	3.07543700	0.25209300	3.16379900
F	3.64754100	1.27998600	3.80439300
F	2.78278000	-0.70233500	4.05524000
F	3.93842100	-0.23661200	2.27097200
C	0.98480500	5.59769500	1.39086500
C	0.59208200	4.78384000	2.66629200
H	1.33889300	4.00363200	2.82848600
H	0.64969600	5.47621800	3.51967300
C	-0.75455100	4.13500500	2.68553800
C	0.75211400	4.74935200	0.09154700
H	1.71819800	4.42287700	-0.30421200
H	0.26413900	5.36211600	-0.66826700
N	-0.02937300	3.51208300	0.24464800
C	-1.22413800	3.25543700	-0.33847900
N	-1.46357900	1.98498300	-0.68638300
C	-2.68021800	1.41944900	-1.15719700
C	-3.88325000	1.53596900	-0.45961400
C	-2.61183300	0.64287600	-2.31776400
C	-5.02424100	0.90107200	-0.95043000
C	-3.75986000	0.01443100	-2.79538200
H	-1.66316200	0.53563700	-2.83114000
C	-4.97382300	0.14558400	-2.12142600
H	-5.86342900	-0.34708600	-2.49444000
C	-3.67931900	-0.86515900	-4.01611400
C	-6.32765900	1.05408200	-0.21194800
F	-3.45728300	-2.15626800	-3.68959600
F	-2.67829300	-0.48660600	-4.84330400
F	-4.82847900	-0.83080700	-4.72774400
F	-7.15233000	0.00223900	-0.42314600
F	-6.99820700	2.16260600	-0.59538900
F	-6.13673600	1.15389000	1.12455900
S	-2.38959200	4.53131200	-0.48080400
H	-3.92693600	2.09638000	0.46501100
C	-1.98079000	4.77269400	2.53703000
H	-0.65598500	1.31976500	-0.73646200
H	-2.15985800	4.74290200	1.20589900
H	-2.86837400	4.22493300	2.85454000

O	0.68338300	1.33907800	3.44183700
H	0.56925800	2.70516300	0.47671600
O	1.97939300	1.87198100	1.35970100
H	-2.03520900	5.85151700	2.68107200
C	3.62161100	-2.91222900	-3.81513400
C	3.22950300	-3.69979400	-2.73774500
C	2.93025000	-3.11893100	-1.49591500
C	3.34263600	-0.90555400	-2.44394900
C	3.69443800	-1.52902000	-3.65289400
C	0.54579700	-3.31138500	0.88235300
C	1.71152100	-4.05833900	0.72537300
C	2.10014700	-4.93320800	1.75244600
C	1.26939700	-5.15754100	2.84531100
C	0.03824300	-4.50273600	2.90891100
C	-0.34542700	-3.55598100	1.94547700
H	4.00550300	-0.90266900	-4.48401100
H	-0.63850800	-4.70195500	3.73463200
C	2.66907500	-4.20480200	-0.45618800
C	2.20089000	-5.37171700	-1.39446700
H	2.31936900	-6.35488000	-0.92899400
H	1.13680700	-5.23508600	-1.61918600
H	4.13124800	-5.46914100	2.33864100
H	3.40596000	-6.56923700	1.17213900
C	2.94703700	-1.73084900	-1.37399100
H	3.86110900	-3.36254900	-4.77515300
H	1.56439500	-5.84200900	3.63680400
C	3.02806300	-5.19776400	-2.68515300
H	3.98959700	-5.72643800	-2.61873200
H	2.51596000	-5.58577900	-3.57295700
C	3.46994300	-5.51207200	1.46559100
C	3.97113300	-4.63191500	0.29764800
H	4.68496700	-5.14294800	-0.35636900
H	4.46003700	-3.73389200	0.69236400
C	-1.67527300	-2.87678500	2.04293100
C	-2.66748100	-3.14208000	1.06449600
C	-1.96525700	-2.02240000	3.13532400
C	-2.45897500	-4.03350900	-0.03720600
C	-3.96345600	-2.51108800	1.17089300
C	-3.27741300	-1.42355000	3.24371000
C	-3.43308300	-4.25580000	-0.97483000
H	-1.50773800	-4.54578300	-0.12383400
C	-4.95298900	-2.76687300	0.16968100
C	-4.23301400	-1.67115700	2.25488100
C	-4.69705800	-3.60832200	-0.87889400

H	-3.24177400	-4.93422000	-1.80184000
H	-5.91346800	-2.26544800	0.25767600
H	-5.20732200	-1.19209200	2.32602800
H	-5.45468300	-3.79244000	-1.63584800
C	3.40279600	0.58720100	-2.35012600
C	4.39989700	1.21083500	-1.56178800
C	2.50364500	1.37249500	-3.11266800
C	5.34334900	0.47189600	-0.77875100
C	4.50410600	2.65237700	-1.55078200
C	2.62849800	2.81233500	-3.10609100
C	6.29877300	1.10402000	-0.02742400
H	5.29419100	-0.61080700	-0.78549300
C	5.51848900	3.27290300	-0.75634500
C	3.62554200	3.41148000	-2.32993600
C	6.38922600	2.52479200	-0.01141900
H	6.99810600	0.51732600	0.56195400
H	5.58407800	4.35874300	-0.76184600
H	3.72756700	4.49557500	-2.34074800
H	7.15481000	3.00867600	0.58915300
C	-1.32370700	-0.87995600	5.19775400
H	-0.56672600	-0.63525800	5.93714900
C	-1.00330500	-1.69552600	4.14488500
H	0.00613300	-2.07559700	4.04869300
C	-2.62803700	-0.32246400	5.31821200
H	-2.86414500	0.31744500	6.16463900
C	-3.57161300	-0.58060400	4.36130000
H	-4.56869600	-0.15125700	4.43143600
C	0.58885000	1.58762200	-4.62083700
H	-0.21461900	1.12583300	-5.18905500
C	0.73538200	3.00508000	-4.63215900
H	0.05579100	3.61208100	-5.22442200
C	1.72515100	3.59517900	-3.89337800
H	1.84483200	4.67653800	-3.89047300
C	1.44185200	0.80278700	-3.88855700
H	1.30548400	-0.27159200	-3.87367000
H	-0.74827200	3.06012200	2.86305600
C	0.21723200	6.93245100	1.28808200
H	0.62409700	7.53446400	0.46679400
H	-0.84683500	6.79285200	1.08245600
H	0.32134200	7.51971100	2.20798900
C	2.49112500	5.91276200	1.50443900
H	2.83575800	6.47398700	0.62750500
H	2.69891500	6.52456500	2.38995500
H	3.08193600	4.99288700	1.57381200

TS-EF-2R-1

l imaginary frequencies

H = -4967.742059

G = -4967.926565

E(M06-2X-DCM) = -4968.519667

O	-2.33554200	-1.42514000	0.42430200
O	-2.93870800	0.72699800	-0.89219800
P	-1.70531600	-0.00179200	-0.10459300
O	-1.23278500	0.72181300	1.12052500
N	-0.64095700	-0.39349600	-1.25107600
S	0.24188000	0.66189200	-2.03891500
C	-0.19459600	0.31976200	-3.82192900
F	0.53208100	1.11498400	-4.61312600
F	0.05583600	-0.95606800	-4.15416200
F	-1.49119600	0.56738000	-4.02427300
C	-0.07774600	-0.44868600	4.35457300
C	-0.20278000	1.10200400	4.20432300
H	-0.99044300	1.31485300	3.47959000
H	-0.52394200	1.49698500	5.17939500
C	1.02456000	1.84199100	3.78137200
C	0.54901300	-1.07175000	3.06245400
H	-0.24262500	-1.53043200	2.46683500
H	1.26563600	-1.84868300	3.32958900
N	1.21621000	-0.13237600	2.13681400
C	2.53161600	-0.14606000	1.82914300
N	2.89279900	0.18550300	0.57756800
C	4.22051900	0.36285000	0.08746000
C	5.11236900	1.27165200	0.66300300
C	4.59093000	-0.36307500	-1.04469400
C	6.38736900	1.41794100	0.12165000
C	5.87098500	-0.20266200	-1.57888400
H	3.88023300	-1.04145400	-1.50273400
C	6.77842500	0.67876100	-0.99784200
H	7.77383900	0.79275900	-1.40954500
C	6.26078800	-1.04367200	-2.76740100
C	7.33542200	2.43402300	0.70385800
F	6.37584100	-2.35211800	-2.42489300
F	7.44287000	-0.66497200	-3.29429100
F	5.33422800	-0.98176200	-3.74493500
F	7.06050600	2.69355400	2.00126700
F	7.26909800	3.61155900	0.04266200
F	8.61736000	2.01514500	0.63332400
S	3.67945400	-0.45301300	3.09169900

H	4.81865800	1.85512500	1.52547000
C	2.24271300	1.87036100	4.45110400
H	2.19430700	0.14649400	-0.18527500
H	2.88589900	0.80457800	3.92807900
H	2.94508000	2.66057400	4.18545100
O	1.67647200	0.27793400	-1.94680000
H	0.53796200	0.26128900	1.46259200
O	-0.07867100	2.08015800	-1.83158000
H	2.26993100	1.56893400	5.49785200
C	-6.38250600	1.67516200	1.28261000
C	-6.20858500	0.40256600	0.74737900
C	-5.08780800	0.10853300	-0.04329500
C	-4.25240700	2.37896800	0.30222900
C	-5.42277000	2.65635500	1.02897600
C	-2.81623200	-2.36430700	-0.48698200
C	-4.07913700	-2.19180800	-1.05326900
C	-4.47401400	-3.03639800	-2.10363100
C	-3.67784000	-4.10773500	-2.49383400
C	-2.48209300	-4.34570500	-1.81537300
C	-2.02016500	-3.48259300	-0.80909900
H	-5.56368900	3.66183100	1.41494300
H	-1.87420000	-5.20749000	-2.07531600
C	-5.23952300	-1.27084700	-0.67571200
C	-6.17216100	-1.95348700	0.38344200
H	-6.72043800	-2.80578800	-0.02966300
H	-5.55327700	-2.32343000	1.20929700
H	-5.79563400	-2.56327500	-3.77256100
H	-6.61323900	-3.26839300	-2.38239000
C	-4.09524300	1.07237700	-0.19940800
H	-7.25679500	1.91063300	1.88449100
H	-3.98558000	-4.76336100	-3.30449400
C	-7.09029100	-0.81920100	0.88981500
H	-7.99540800	-0.73158900	0.27243700
H	-7.42825500	-0.97724200	1.92050600
C	-5.80137800	-2.58854400	-2.67689100
C	-5.98297600	-1.18860400	-2.05083500
H	-7.03121700	-0.89303200	-1.94201200
H	-5.48555800	-0.43660500	-2.67382800
C	-0.75790900	-3.82085400	-0.07547200
C	-0.83867900	-4.27806700	1.26515400
C	0.49484700	-3.78131000	-0.73487200
C	-2.07796400	-4.39278200	1.97535800
C	0.36507300	-4.68047300	1.95911700
C	1.68924100	-4.19686900	-0.03198200

C	-2.12499000	-4.84488300	3.26898400
H	-2.99739400	-4.12444900	1.46782600
C	0.27392300	-5.13935100	3.31137000
C	1.59341800	-4.62786600	1.29381800
C	-0.93291200	-5.21876100	3.95355500
H	-3.08202900	-4.92763100	3.77731800
H	1.19091000	-5.43734300	3.81491200
H	2.49501500	-4.94008700	1.81746900
H	-0.98884500	-5.57909700	4.97735700
C	-3.24027200	3.45317300	0.06032300
C	-3.01510100	3.92420000	-1.25695200
C	-2.54404600	4.03202300	1.14981800
C	-3.72505000	3.42295500	-2.39443000
C	-2.05013100	4.97467400	-1.48511200
C	-1.59852400	5.09854100	0.90767500
C	-3.48039900	3.89775800	-3.65590900
H	-4.47611500	2.65533700	-2.24825100
C	-1.81992600	5.43839500	-2.81758000
C	-1.37067400	5.53247900	-0.40014600
C	-2.50946600	4.91509400	-3.87654600
H	-4.03396300	3.49561900	-4.50026300
H	-1.07997500	6.22078500	-2.96818000
H	-0.64971600	6.32789100	-0.57792000
H	-2.32414900	5.27370000	-4.88537300
C	1.86942300	-3.29525800	-2.69470100
H	1.95296400	-2.91745100	-3.70902900
C	0.64359200	-3.32479000	-2.08314400
H	-0.22920300	-2.96284300	-2.60959700
C	3.04073300	-3.72134200	-2.00446000
H	4.00617600	-3.68026100	-2.50140800
C	2.94917400	-4.15375300	-0.70816200
H	3.83583400	-4.47300600	-0.16521900
C	-2.05755100	4.21147600	3.54154600
H	-2.23028300	3.87751800	4.56181600
C	-1.13951700	5.27322000	3.29747100
H	-0.62376700	5.74472100	4.13016200
C	-0.91435800	5.69349100	2.01407100
H	-0.21238400	6.49872500	1.80920000
C	-2.72420600	3.60722300	2.50617200
H	-3.40347500	2.78769600	2.70940600
H	0.93340800	2.43317300	2.87204000
C	0.74114800	-0.86115500	5.59539300
H	0.67980100	-1.94716900	5.73216800
H	1.80125600	-0.61110300	5.50969600

H	0.34354000	-0.39190800	6.50326500
C	-1.50857400	-1.00264200	4.51596900
H	-1.49284900	-2.09584200	4.58795500
H	-1.97714600	-0.61227900	5.42744600
H	-2.13121400	-0.73029200	3.65777000

TS-EF-2R-2

1 imaginary frequencies

H = -4967.743966

G = -4967.926010

E(M06-2X-DCM) = -4968.522122

O	-1.89572900	-1.67284800	0.22177500
O	-3.12516700	0.36158400	-0.82592000
P	-1.63645900	-0.15880800	-0.38061000
O	-1.04684900	0.62290000	0.75723400
N	-0.91027900	-0.32355100	-1.80287500
S	0.20690600	0.57510100	-2.46514500
C	-0.56228700	2.26020000	-2.73150100
F	0.29229200	3.04543700	-3.39590200
F	-1.69155200	2.15120800	-3.43398600
F	-0.83893300	2.82773400	-1.54828900
C	-0.20664100	-0.76072700	4.22235400
C	-0.39453700	0.78865400	4.17057500
H	-1.14333200	1.01831500	3.40919200
H	-0.79944900	1.10246000	5.14409300
C	0.82165100	1.60842800	3.87690700
C	0.53293300	-1.25060200	2.93309600
H	-0.18735500	-1.72147400	2.26076200
H	1.28883600	-1.99250200	3.19132900
N	1.17291400	-0.19791500	2.12015500
C	2.49565300	-0.10859000	1.86641900
N	2.85738300	0.37875800	0.66851300
C	4.17562700	0.64451300	0.19859500
C	5.06608500	1.46947500	0.89113400
C	4.54189800	0.09116900	-1.02984500
C	6.33594700	1.70164800	0.36691700
C	5.81926000	0.33030400	-1.54026400
H	3.83613000	-0.52468200	-1.57662000
C	6.72493200	1.12856100	-0.84591500
H	7.71756600	1.30453000	-1.24208300
C	6.22059800	-0.34772900	-2.82575300
C	7.27765600	2.63671700	1.08055400
F	6.40855300	-1.67912100	-2.63781300
F	7.37188500	0.14848000	-3.32366800

F	5.27206400	-0.22095900	-3.77447500
F	7.02882000	2.68442500	2.40792200
F	7.16994500	3.90124600	0.61337800
F	8.56571500	2.26554800	0.91877500
S	3.62120300	-0.47664700	3.13364600
H	4.77639100	1.92082800	1.83048000
C	1.99853000	1.63761800	4.61660000
H	2.13349100	0.44354700	-0.06991300
H	2.73308700	0.65319100	4.04145300
H	2.67157700	2.47999700	4.45650100
O	0.52868300	0.09537000	-3.80787300
H	0.50746700	0.19245200	1.42075900
O	1.35115600	0.88872400	-1.56350300
H	1.98695400	1.25036100	5.63474100
C	-6.15926000	0.60446600	2.04454300
C	-5.86494100	-0.60568800	1.42432300
C	-4.89784800	-0.67330200	0.40963800
C	-4.46197400	1.71552800	0.67463900
C	-5.48275100	1.75563100	1.63971700
C	-2.37750300	-2.68856800	-0.60366200
C	-3.73743000	-2.73707400	-0.90357000
C	-4.18686700	-3.62905500	-1.88986700
C	-3.31456700	-4.54367800	-2.47036500
C	-1.98725700	-4.58024500	-2.04067000
C	-1.48705700	-3.65763100	-1.10817700
H	-5.73466300	2.71444200	2.08366400
H	-1.30824100	-5.32659100	-2.44276800
C	-4.93425100	-2.04641200	-0.25441300
C	-5.49069100	-2.90775900	0.93159700
H	-5.95495400	-3.83806000	0.59033700
H	-4.65729100	-3.17410000	1.59242500
H	-5.87881000	-3.36846100	-3.24099800
H	-6.26732300	-4.23299800	-1.75792800
C	-4.15408600	0.46470100	0.10218400
H	-6.91753800	0.66162400	2.82159600
H	-3.66061800	-5.23639400	-3.23327600
C	-6.46605900	-1.97126100	1.67651900
H	-7.48180200	-2.04013600	1.26242900
H	-6.54677300	-2.20610200	2.74423500
C	-5.65941600	-3.41437500	-2.16821500
C	-5.94900900	-2.07942600	-1.44604300
H	-6.98741200	-1.98077700	-1.11409900
H	-5.72973900	-1.24061800	-2.11634400
C	-0.07636000	-3.79135600	-0.62073400

C	0.15247100	-4.28319200	0.69010400
C	1.01860100	-3.52616500	-1.47845400
C	-0.90903200	-4.63960800	1.58488400
C	1.50778400	-4.47426000	1.15792400
C	2.36959900	-3.73447400	-1.00126800
C	-0.65616300	-5.12126800	2.84427500
H	-1.93368200	-4.53935900	1.24520100
C	1.72880100	-4.96791800	2.48277700
C	2.57679500	-4.19092300	0.30304500
C	0.68142900	-5.28145000	3.30769000
H	-1.48386900	-5.39795900	3.49241300
H	2.75564300	-5.10090900	2.81566700
H	3.59458400	-4.34282400	0.65728100
H	0.86445900	-5.66795900	4.30684400
C	-3.78855400	2.98338400	0.25220200
C	-3.99533600	3.48328100	-1.05850600
C	-3.01063700	3.72195700	1.17691400
C	-4.81417200	2.81712700	-2.02556600
C	-3.38250300	4.73137600	-1.45272000
C	-2.41916100	4.97802500	0.77335200
C	-4.98749300	3.32370500	-3.28674400
H	-5.30934500	1.89410600	-1.74775200
C	-3.58373600	5.22306500	-2.78010900
C	-2.61328100	5.44296400	-0.52891000
C	-4.35846500	4.53934800	-3.67692700
H	-5.61193900	2.79260300	-4.00001500
H	-3.10463700	6.15845500	-3.05950400
H	-2.15945800	6.38505700	-0.82982100
H	-4.50161900	4.92133100	-4.68395600
C	1.93266600	-2.79422700	-3.62112500
H	1.77488100	-2.39070400	-4.61559300
C	0.85259100	-3.03925400	-2.81410100
H	-0.14565100	-2.82248200	-3.17291500
C	3.25902100	-3.01084900	-3.15154400
H	4.10326200	-2.79192900	-3.79815000
C	3.46887600	-3.46099600	-1.87483900
H	4.47883500	-3.61107400	-1.50072700
C	-2.04161200	4.03922400	3.40128000
H	-1.89880400	3.69119000	4.42153200
C	-1.46990200	5.28059700	2.99955400
H	-0.89413000	5.86642500	3.71124500
C	-1.65067500	5.72737600	1.71886300
H	-1.21681000	6.67026800	1.39417800
C	-2.77411400	3.28485900	2.52043400

H	-3.19518000	2.33868300	2.83984500
H	0.74924400	2.27073600	3.01640500
C	0.55518400	-1.22492300	5.48094500
H	0.54518700	-2.31972100	5.53390500
H	1.60378100	-0.91780700	5.48024400
H	0.08007300	-0.84509000	6.39345000
C	-1.61494600	-1.38986000	4.25197900
H	-1.54493600	-2.48328600	4.24509400
H	-2.15863200	-1.09240900	5.15670000
H	-2.20039100	-1.08654200	3.37752100

INT-8

0 imaginary frequencies

H = -4967.796089

G = -4967.976330

E(M06-2X-DCM) = -4968.585630

O	1.55217500	-2.11807700	-0.07204000
O	3.12168100	-0.12694100	0.46416000
P	1.56222900	-0.49531900	0.13201800
O	0.74592300	-0.05030100	1.31239400
C	2.58212700	-4.38996200	3.29495700
C	3.56595900	-3.87805200	2.45538200
C	3.21660200	-3.18741400	1.28537800
C	0.85406900	-3.45862400	1.83187000
C	1.24111100	-4.20482400	2.95833400
C	4.12983000	-0.44107400	-0.45453800
C	4.62420500	-1.74476900	-0.50942500
C	5.51185900	-2.09680300	-1.53905400
C	5.98672800	-1.13917900	-2.42777200
C	5.57970100	0.18498500	-2.27315300
C	4.64317600	0.56505500	-1.29736300
H	0.46268000	-4.62602600	3.58774400
H	5.97629300	0.95334700	-2.93018900
C	4.45912600	-2.92469100	0.44512300
C	5.55095100	-2.89833600	1.56866600
H	5.56373600	-1.90071400	2.02283800
H	6.55417900	-3.10140600	1.18138000
H	6.82923100	-3.76760100	-1.11979000
H	5.76122200	-4.04284600	-2.49168000
C	1.87465100	-2.92497400	1.02337900
H	2.84803100	-4.93446500	4.19755700
H	6.67657400	-1.41024200	-3.22295600
C	5.07064800	-3.93652800	2.60660100
H	5.40041300	-3.70004400	3.62475300

H	5.45532900	-4.94009300	2.37681100
C	5.81559000	-3.57863000	-1.50037600
C	4.74063900	-4.11530800	-0.53184900
H	3.82187100	-4.33962400	-1.08570500
H	5.04353800	-5.02516500	-0.00435600
C	4.30590600	2.01834600	-1.16601100
C	3.61218100	2.68594500	-2.20435300
C	4.80497000	2.74962600	-0.05803600
C	3.07630800	2.00073900	-3.34166200
C	3.41865900	4.11736500	-2.13029600
C	4.58725900	4.17763700	0.01204400
C	2.42151900	2.67726300	-4.33606600
H	3.16162700	0.92272100	-3.38973100
C	2.73620300	4.78575100	-3.19494100
C	3.90516700	4.82098700	-1.02514100
C	2.25557300	4.08968700	-4.27031500
H	2.00115700	2.12676900	-5.17246300
H	2.60785400	5.86375400	-3.12729900
H	3.76221400	5.89915500	-0.97741600
H	1.73439200	4.60756700	-5.07090600
C	-0.59938500	-3.29556900	1.52249500
C	-1.43460000	-2.57909900	2.41347100
C	-1.15143600	-3.93080600	0.38242500
C	-0.93286400	-1.89029100	3.56616600
C	-2.85708200	-2.51774400	2.16494200
C	-2.57154600	-3.83758400	0.13177900
C	-1.77344000	-1.22785200	4.42371400
H	0.13500300	-1.89082000	3.74902400
C	-3.69816600	-1.81449500	3.08438900
C	-3.38581000	-3.14310000	1.03216900
C	-3.17820700	-1.19240900	4.18703400
H	-1.36666500	-0.72299100	5.29651500
H	-4.76666300	-1.78601800	2.88470800
H	-4.45461300	-3.08409100	0.84179100
H	-3.82846700	-0.66293600	4.87745500
C	6.03845000	2.88177400	2.05125200
H	6.61175600	2.39425500	2.83528900
C	5.56006600	2.14496000	0.99864400
H	5.76200100	1.08087200	0.95427700
C	5.79826200	4.28370000	2.12721200
H	6.18543900	4.85263800	2.96827100
C	5.09501400	4.90862500	1.13227700
H	4.91932400	5.98160000	1.16745900
C	-0.93326800	-5.29575400	-1.63286700

H	-0.31170300	-5.86858200	-2.31595900
C	-2.32902500	-5.17953800	-1.88659300
H	-2.75874900	-5.65647900	-2.76324800
C	-3.12354600	-4.47379500	-1.02466200
H	-4.18971000	-4.37564300	-1.20488600
C	-0.36701200	-4.69671500	-0.53837800
H	0.69616800	-4.80596300	-0.35844800
C	1.06758200	3.08191900	2.84466600
C	1.11376000	3.27614100	1.29829500
H	1.52106300	4.25166900	1.01888000
H	1.75904300	2.52001200	0.84659300
C	-0.31385200	3.11682600	0.75850900
C	-0.28564400	2.36182700	3.09963300
H	-0.99637700	2.98336200	3.64127400
H	-0.18721100	1.40493100	3.61410000
N	-0.89536700	2.06081100	1.74268500
C	-2.40095300	1.94073100	1.70139300
N	-2.78027100	1.28921200	0.59038100
C	-4.10236800	1.07351300	0.10859700
C	-5.13968000	1.99588400	0.28691200
C	-4.32323100	-0.08724400	-0.64446400
C	-6.39376300	1.73616100	-0.26384700
C	-5.58644600	-0.32943500	-1.18315000
H	-3.50944100	-0.78059700	-0.82025700
C	-6.63175600	0.57343000	-0.99472600
H	-7.60714500	0.38478900	-1.42645500
C	-5.83422200	-1.61112400	-1.93590600
C	-7.51992100	2.70902100	-0.02197600
F	-4.75245300	-2.00734300	-2.63165200
F	-6.86415200	-1.49724100	-2.79945700
F	-6.14964000	-2.62798200	-1.08637400
F	-8.19690000	2.41072100	1.10944100
F	-8.41488300	2.69585700	-1.03312600
F	-7.06884600	3.97522700	0.10910700
S	-3.34309500	2.59792400	2.88716500
H	-4.97728400	2.91047800	0.83726800
H	-2.06814400	0.79388600	0.02264400
H	-0.44069300	1.14702400	1.45834700
C	-1.14262700	4.39593600	0.71172300
H	-1.25544200	4.86978000	1.69020100
H	-2.13884500	4.22257800	0.29574000
H	-0.62676800	5.09679900	0.04773600
N	1.27993900	0.13518600	-1.32727300
S	-0.14978800	0.25808200	-1.98369700

O	-0.38712800	1.58281600	-2.56988700
O	-1.25547700	-0.28766700	-1.13735200
C	-0.07106700	-0.92083800	-3.42932900
F	0.90376600	-0.54683200	-4.26899100
F	-1.23592500	-0.90039000	-4.08320500
F	0.17339400	-2.15992700	-3.00172100
C	2.24892900	2.22304900	3.33044900
H	3.20021200	2.71053700	3.09333800
H	2.20390800	2.08712600	4.41863500
H	2.24040400	1.23896000	2.85556000
C	1.09420700	4.43224700	3.58880200
H	0.99288700	4.28353900	4.67072800
H	2.04798400	4.94132100	3.41092900
H	0.28912300	5.10248700	3.26829200
H	-0.32122500	2.65075700	-0.22968400

TS-PT-2

l imaginary frequencies

H = -4967.788320

G = -4967.967693

E(M06-2X-DCM) = -4968.573471

O	-1.31439800	2.18798100	-0.18782500
O	-2.91392300	0.20932500	0.35537000
P	-1.37662800	0.59077400	-0.00170400
O	-0.57803100	0.19762500	1.26263600
C	-2.60017800	4.71584800	2.89452900
C	-3.51644200	4.13779000	2.02180000
C	-3.07657200	3.34785300	0.94934800
C	-0.75985900	3.66533200	1.66450100
C	-1.23716400	4.50191400	2.68887000
C	-3.91564300	0.45040900	-0.60752400
C	-4.35871300	1.75523800	-0.82214400
C	-5.17658300	2.01718100	-1.93411300
C	-5.64283500	0.98019700	-2.73400000
C	-5.32100200	-0.33302500	-2.39298400
C	-4.45484100	-0.63288400	-1.32848500
H	-0.51077900	4.97635300	3.34167900
H	-5.73675200	-1.15866100	-2.96283300
C	-4.24190500	3.02093000	0.02607100
C	-5.43063900	3.10549900	1.04596800
H	-5.50259700	2.15168500	1.58162200
H	-6.39113700	3.28406000	0.55322700
H	-6.46460200	3.75587700	-1.80114100
H	-5.28036400	3.85667400	-3.09898200

C	-1.72015400	3.06814800	0.82958300
H	-2.93544100	5.33772800	3.72071000
H	-6.27484300	1.18212800	-3.59492700
C	-5.02682100	4.22416700	2.03076400
H	-5.45157500	4.07945700	3.03058400
H	-5.37072800	5.20802900	1.68216000
C	-5.43041300	3.50276500	-2.07274700
C	-4.41894800	4.11418400	-1.07925200
H	-3.45544200	4.27048200	-1.57747100
H	-4.74126200	5.07480900	-0.66607200
C	-4.27056300	-2.07160900	-0.94831000
C	-3.56435800	-2.96180900	-1.79189700
C	-4.94781900	-2.56256400	0.19833400
C	-2.85559800	-2.52334700	-2.95518400
C	-3.53979800	-4.37472300	-1.48219600
C	-4.90239500	-3.97562300	0.50284100
C	-2.18340200	-3.41021600	-3.75482800
H	-2.83310700	-1.46601000	-3.18350600
C	-2.83241400	-5.26714500	-2.34772400
C	-4.20751700	-4.84110000	-0.34702400
C	-2.17501800	-4.80204900	-3.45425200
H	-1.63646000	-3.04605400	-4.61884100
H	-2.83057300	-6.32703800	-2.10382600
H	-4.19146200	-5.90579900	-0.12148600
H	-1.63851700	-5.48881500	-4.10323000
C	0.71033900	3.47782100	1.47603500
C	1.47820400	2.85555100	2.49019900
C	1.33825600	3.99199000	0.31457800
C	0.90331600	2.31508100	3.68667800
C	2.91041800	2.74516300	2.32924900
C	2.76419000	3.83154000	0.14783100
C	1.68599600	1.76348700	4.66764300
H	-0.17310500	2.34417300	3.81064900
C	3.68869300	2.16001400	3.37625700
C	3.50954100	3.21349500	1.15635500
C	3.10026900	1.69319700	4.51978000
H	1.22342600	1.36740400	5.56803600
H	4.76480800	2.09080300	3.23848000
H	4.58208300	3.09391200	1.02305900
H	3.70313000	1.25032700	5.30726000
C	-6.36172900	-2.23511900	2.16839200
H	-6.93779500	-1.57407100	2.81030500
C	-5.71666800	-1.72586400	1.07108900
H	-5.79328900	-0.66739700	0.85055700

C	-6.29159800	-3.62352200	2.47610600
H	-6.80813800	-4.00914100	3.35073400
C	-5.58426500	-4.46558800	1.66088400
H	-5.53345200	-5.53088300	1.87399100
C	1.27103900	5.17930600	-1.82006800
H	0.70659500	5.71509400	-2.57888600
C	2.66975000	4.98418500	-1.99587600
H	3.15815100	5.35996900	-2.89077500
C	3.39309600	4.33074900	-1.03594600
H	4.46059600	4.17311200	-1.15496500
C	0.62988800	4.69990400	-0.70824200
H	-0.43485500	4.86827200	-0.59147500
C	-1.25977600	-2.86909100	2.94156000
C	-1.35080600	-3.15259300	1.41136600
H	-1.78159500	-4.13422700	1.19713700
H	-1.99945500	-2.41526400	0.93162000
C	0.06963500	-3.04231600	0.83622000
C	0.14984300	-2.24305300	3.11961300
H	0.83452100	-2.91995000	3.63480800
H	0.14335000	-1.30201600	3.67328000
N	0.67988800	-1.97300900	1.73963000
C	2.11454800	-1.77294800	1.65404100
N	2.54782800	-1.60754700	0.37967800
C	3.90489700	-1.37556400	0.00077200
C	4.89843300	-2.31167100	0.30020700
C	4.21551700	-0.22318500	-0.72245200
C	6.20821000	-2.08315400	-0.11430900
C	5.53584800	-0.00799700	-1.12999800
H	3.43627900	0.49338300	-0.96152000
C	6.53631600	-0.92879800	-0.82802100
H	7.55772200	-0.75298300	-1.14435800
C	5.89577900	1.27134700	-1.83785800
C	7.26860800	-3.12073100	0.14518500
F	4.88950300	1.72942200	-2.60482000
F	6.98233100	1.12323000	-2.62653300
F	6.19627300	2.26062800	-0.95042400
F	8.48255100	-2.55739200	0.33216100
F	7.39064800	-3.97638100	-0.89716600
F	6.99032400	-3.86581900	1.23545400
S	3.09278700	-1.72034600	2.99516300
H	4.65078000	-3.20521400	0.85880100
H	1.88112500	-1.55100700	-0.39476000
H	0.00629000	-0.75990300	1.38729100
C	0.85459000	-4.35669700	0.84645600

H	0.95063400	-4.77583800	1.85261300
H	1.85779500	-4.23225700	0.42930100
H	0.32424500	-5.08457600	0.22352900
N	-1.00627500	-0.10451000	-1.38468600
S	0.42142000	-0.00350400	-2.09787700
O	1.06031100	-1.33799200	-2.16173700
O	1.26584300	1.11505500	-1.65490800
C	-0.05386400	0.40249600	-3.85787100
F	-0.81699200	-0.55961100	-4.39170700
F	1.06166300	0.51816400	-4.57929700
F	-0.72465000	1.55440400	-3.88788000
C	-2.36643200	-1.89966900	3.39630300
H	-3.35743100	-2.32528800	3.20422700
H	-2.28860400	-1.70314800	4.47311500
H	-2.30294800	-0.94321600	2.87009800
C	-1.37196400	-4.16551200	3.76744400
H	-1.22461100	-3.96375900	4.83555300
H	-2.36689800	-4.60950100	3.64644500
H	-0.63048500	-4.91330300	3.46486000
H	0.04239300	-2.65038500	-0.18370600

TS-1-1-3S

l imaginary frequencies

H = -4967.752016

G = -4967.931576

E(M06-2X-DCM) = -4968.525288

C	1.11210800	-2.39211700	-4.38532000
C	0.38159100	-1.16371000	-5.05837500
H	1.13387000	-0.60830900	-5.62928200
H	-0.36134900	-1.57261500	-5.75491300
C	-0.32107400	-0.24111200	-4.13367000
C	0.09902500	-3.18772800	-3.54244800
H	0.61578400	-4.04534200	-3.08914200
H	-0.70545000	-3.57284600	-4.17226500
N	-0.51718900	-2.39150800	-2.48844100
C	-1.85734400	-2.48317100	-2.14842100
N	-2.07789500	-1.99455400	-0.89164300
C	-3.21412900	-1.90327900	-0.07447200
C	-4.53614600	-2.16888600	-0.45997000
C	-2.95782600	-1.50380300	1.25025100
C	-5.56227000	-2.04030000	0.47814100
C	-3.99449400	-1.38987200	2.16889200
H	-1.93988100	-1.28245200	1.55478100
C	-5.31154300	-1.66142700	1.79592300

H	-6.11892900	-1.58438500	2.51389300
C	-3.69146200	-0.89226600	3.55562100
C	-6.98894700	-2.23858600	0.03530000
F	-4.61355100	-1.28981700	4.45463200
F	-3.66105900	0.46879200	3.60230100
F	-2.48242600	-1.31256200	3.99569700
F	-7.54806100	-1.06522700	-0.36065600
F	-7.76277700	-2.71611900	1.03515200
F	-7.09016500	-3.09049600	-1.00303100
S	-3.02127400	-3.06528300	-3.21799400
C	1.62613600	-3.30271700	-5.51479700
H	2.33790000	-2.76979600	-6.15502300
H	2.14491300	-4.17249900	-5.09609400
H	0.80671700	-3.66827600	-6.14467500
C	2.30027300	-1.90896800	-3.53694500
H	2.82900400	-2.76665300	-3.10605500
H	3.01667400	-1.34813600	-4.14808000
H	2.00064400	-1.26197300	-2.70908800
H	-4.75237900	-2.47582800	-1.47288100
C	0.20490200	0.97049700	-3.66037700
H	-1.23878000	-1.61261300	-0.43949200
H	1.05956800	1.38075400	-4.20329700
H	-0.53667000	1.71413800	-3.36019900
H	0.10358000	-2.11407200	-1.72629400
H	0.76650300	0.80957800	-2.57260900
O	-0.22500000	1.28241800	0.75259800
O	2.19122500	0.38720800	1.19166000
P	0.98131200	0.39517100	0.10486500
O	0.38863400	-0.95657200	-0.14712500
C	0.45440400	5.18284400	2.13281100
C	0.87647500	4.08667100	2.87634800
C	0.56866400	2.78082000	2.46545900
C	-0.55310900	3.67601700	0.48706400
C	-0.29067900	4.96791700	0.97575400
C	1.95017200	-0.30935400	2.39122300
C	1.25678300	0.33785700	3.40984700
C	0.85866800	-0.39963300	4.53692000
C	1.23737600	-1.72938000	4.68496900
C	2.02254900	-2.32575900	3.69825700
C	2.38246900	-1.64281200	2.52498900
H	-0.67218200	5.81527600	0.41440700
H	2.35204600	-3.35403200	3.81571900
C	0.89288400	1.80635100	3.59584700
C	2.05052700	2.58260800	4.30829700

H	2. 18688200	2. 26425000	5. 34656100
H	2. 98599600	2. 38968100	3. 77104600
H	-0. 89200500	-0. 08285300	5. 78864800
H	0. 56157800	0. 73986400	6. 35632900
C	-0. 05342600	2. 58905500	1. 23263600
H	0. 68142400	6. 19549100	2. 45596700
H	0. 93296400	-2. 29944300	5. 55891600
C	1. 66580300	4. 07079100	4. 16684900
H	1. 05280600	4. 41037900	5. 01336500
H	2. 54059000	4. 72964000	4. 12753000
C	0. 00583500	0. 44740900	5. 45465200
C	-0. 32771800	1. 66743700	4. 56973300
H	-0. 50794700	2. 58294500	5. 14112100
H	-1. 23016200	1. 45547900	3. 98684100
C	3. 23428000	-2. 33770100	1. 50799100
C	4. 60481200	-1. 99528700	1. 40186600
C	2. 70337500	-3. 39602900	0. 73231600
C	5. 22168700	-1. 00182800	2. 22797000
C	5. 44398200	-2. 69239100	0. 45392500
C	3. 56117200	-4. 10304800	-0. 19281500
C	6. 55267300	-0. 70000500	2. 10771500
H	4. 61717500	-0. 48377300	2. 96387200
C	6. 82448400	-2. 33486200	0. 34785300
C	4. 89956400	-3. 72143000	-0. 31915800
C	7. 36676500	-1. 36633600	1. 14847000
H	6. 99448300	0. 05799700	2. 74872000
H	7. 43772700	-2. 86147200	-0. 37961200
H	5. 53944500	-4. 25270000	-1. 02109600
H	8. 41847600	-1. 10746600	1. 06222200
C	-1. 39641200	3. 53361100	-0. 74216300
C	-2. 68363000	2. 94341500	-0. 64869500
C	-0. 96248500	4. 09813600	-1. 96997600
C	-3. 22263100	2. 43246000	0. 57542900
C	-3. 52870100	2. 87863900	-1. 82109100
C	-1. 83726300	4. 06197100	-3. 12314100
C	-4. 47057800	1. 86893800	0. 62815200
H	-2. 63358700	2. 50335700	1. 48212100
C	-4. 81438000	2. 25843700	-1. 72850600
C	-3. 08535200	3. 44104900	-3. 02085400
C	-5. 27510400	1. 75896400	-0. 54108400
H	-4. 84535500	1. 49486900	1. 57473200
H	-5. 42103400	2. 19804100	-2. 62905900
H	-3. 73482000	3. 40769200	-3. 89366500
H	-6. 24319800	1. 27027400	-0. 48463000

C	0.86104300	-4.86868100	0.08410600
H	-0.17788900	-5.17216000	0.18092800
C	1.33692800	-3.81775300	0.82472900
H	0.67385200	-3.28456200	1.49490700
C	1.71531700	-5.57198100	-0.81467400
H	1.32402800	-6.41180700	-1.38288000
C	3.02384600	-5.19122700	-0.95159600
H	3.68799200	-5.72118200	-1.63078700
C	0.70849500	5.24687900	-3.33667400
H	1.70081000	5.67650500	-3.43632400
C	-0.16904300	5.23653800	-4.45708100
H	0.14969500	5.68177600	-5.39577300
C	-1.40276600	4.65339800	-4.35138600
H	-2.08063700	4.62665300	-5.20163700
C	0.32736300	4.69971900	-2.13885300
H	1.02429200	4.69443000	-1.30976600
N	1.60265800	1.06527900	-1.24941300
S	2.83450400	2.11187800	-1.44779300
C	4.39954900	1.08786500	-1.19202800
O	2.89737500	3.15438400	-0.42049700
O	2.86701000	2.46588600	-2.86983500
F	4.20005900	-0.18601300	-1.55737300
F	5.36713300	1.60866700	-1.95171500
F	4.77776000	1.12656600	0.08178200
H	-1.34651100	-0.49725900	-3.87783000

TS-1-1-3R

l imaginary frequencies

H = -4967.742182

G = -4967.923832

E(M06-2X-DCM) = -4968.523086

C	0.21336700	3.45382400	-3.85856800
C	0.26604500	2.10332500	-4.69100800
H	1.11783100	2.19759300	-5.37555200
H	-0.65927700	2.04577500	-5.27448400
C	0.42707000	0.85942100	-3.90720100
C	-1.08647300	3.46950500	-3.02836300
H	-1.06022300	4.33085600	-2.34642700
H	-1.95156000	3.59436200	-3.68182900
N	-1.31504500	2.24622600	-2.26817500
C	-2.58789400	1.69729800	-2.10313200
N	-2.56935000	0.68871000	-1.18715000
C	-3.60530700	-0.01033500	-0.54103000
C	-4.90363300	-0.18732300	-1.03763800

C	-3.26155200	-0.58662600	0.69545000
C	-5.83288300	-0.91705500	-0.29120400
C	-4.20420500	-1.30364200	1.42465500
H	-2.25899400	-0.45158100	1.08592400
C	-5.50254300	-1.47699600	0.94034300
H	-6.23628600	-2.03456700	1.50944400
C	-3.84533700	-1.81944700	2.79151300
C	-7.19995700	-1.16276400	-0.87707100
F	-2.52812100	-2.11582300	2.89381100
F	-4.11189800	-0.90458000	3.75933800
F	-4.53736200	-2.93278400	3.11189300
F	-8.12127700	-1.40735300	0.08134300
F	-7.63491200	-0.11227400	-1.60229400
F	-7.19616100	-2.23689800	-1.70229300
S	-3.92301800	2.22707400	-2.97555900
C	0.14526200	4.60822200	-4.87628800
H	1.07320100	4.67707200	-5.45462400
H	0.01042400	5.56255900	-4.35468100
H	-0.68971600	4.48527000	-5.57567900
C	1.45986200	3.63054900	-2.97811500
H	1.45351400	4.62766500	-2.52478600
H	2.38189500	3.54308000	-3.56336100
H	1.52838200	2.90912400	-2.16095700
H	-5.18350300	0.24827100	-1.98582100
C	1.66226800	0.35047200	-3.45701000
H	-1.63411900	0.37453000	-0.88931100
H	2.55852800	0.77904900	-3.90923000
H	1.68470800	-0.73686700	-3.33961200
H	-0.69568300	2.11224900	-1.47441900
H	1.77300600	0.65793500	-2.29645300
O	1.99233600	-1.42544000	0.55268400
O	0.49819600	0.49359800	1.45980700
P	1.12249500	-0.13354500	0.09120700
O	-0.05939800	-0.41823700	-0.77792700
C	-0.09749200	-4.59000000	2.32313100
C	0.33471300	-3.51341400	3.08990800
C	1.09855600	-2.48256300	2.51792500
C	0.92893400	-3.59211800	0.34368200
C	0.22456300	-4.63409900	0.96598400
C	1.25615300	0.91687600	2.55666200
C	1.83275700	-0.02470500	3.40490400
C	2.74205700	0.41914300	4.37815800
C	2.94534400	1.77799600	4.59372500
C	2.22565600	2.70260500	3.83706100

C	1. 37791100	2. 30008100	2. 79253300
H	-0. 09399500	-5. 47694400	0. 35940600
H	2. 33140400	3. 76454400	4. 03709500
C	1. 57519800	-1. 51947900	3. 60159500
C	0. 44133900	-1. 73449000	4. 66511300
H	0. 75134600	-1. 43752200	5. 67126900
H	-0. 42405500	-1. 12351500	4. 38509300
H	3. 01820800	-0. 85952600	6. 11125300
H	4. 47457600	-0. 65679400	5. 14326700
C	1. 33550200	-2. 51075200	1. 14814900
H	-0. 68575600	-5. 38732800	2. 76986700
H	3. 63938100	2. 12119100	5. 35661900
C	0. 06483900	-3. 22617100	4. 54943800
H	-0. 97829700	-3. 41749500	4. 82201600
H	0. 68863500	-3. 85235900	5. 20241000
C	3. 38519700	-0. 75767600	5. 08051300
C	2. 95128900	-1. 95465700	4. 20458900
H	3. 66587600	-2. 09313500	3. 38525400
H	2. 88563600	-2. 89687500	4. 75770000
C	0. 59473900	3. 31887200	2. 02454100
C	1. 26015600	4. 33214200	1. 28751900
C	-0. 82372800	3. 31441300	2. 10299400
C	2. 68527200	4. 37997500	1. 14236500
C	0. 48672200	5. 36478700	0. 63174800
C	-1. 58317100	4. 32609000	1. 40257200
C	3. 29706400	5. 38581700	0. 43998900
H	3. 28519600	3. 58780500	1. 57271000
C	1. 16688400	6. 40464700	-0. 07798900
C	-0. 90880700	5. 32675400	0. 69648700
C	2. 53314200	6. 42233000	-0. 16727500
H	4. 37793200	5. 38386900	0. 33415400
H	0. 56848300	7. 18511900	-0. 54314400
H	-1. 48592700	6. 10233300	0. 19609300
H	3. 03824300	7. 21882700	-0. 70733000
C	1. 23699700	-3. 66195900	-1. 12036400
C	0. 20371500	-3. 49493900	-2. 07367600
C	2. 55998100	-3. 94084900	-1. 54261700
C	-1. 15494300	-3. 22256300	-1. 70907500
C	0. 51400300	-3. 58479100	-3. 48377600
C	2. 85817800	-4. 01881800	-2. 95463600
C	-2. 13162900	-3. 06795700	-2. 65751100
H	-1. 40337200	-3. 12430000	-0. 65926600
C	-0. 53488800	-3. 41250800	-4. 44231700
C	1. 83035900	-3. 83408500	-3. 88445200

C	-1.82137200	-3.16519600	-4.04487600
H	-3.15310200	-2.85902200	-2.35235800
H	-0.28484800	-3.49210800	-5.49800300
H	2.05811500	-3.90117900	-4.94674100
H	-2.61063000	-3.04303000	-4.78183500
C	-2.93283800	2.36228900	2.90316300
H	-3.45989100	1.60665500	3.47797100
C	-1.56231400	2.35640500	2.87066300
H	-1.02038400	1.61482100	3.44556700
C	-3.67289100	3.33916400	2.17855200
H	-4.75869900	3.32454200	2.20800800
C	-3.01246100	4.29718000	1.45884200
H	-3.56350300	5.05890300	0.91261200
C	4.90220200	-4.44611800	-1.06401900
H	5.69716000	-4.62037700	-0.34409100
C	5.19393700	-4.50221500	-2.45638800
H	6.20722500	-4.71495900	-2.78593400
C	4.19757600	-4.29553700	-3.37168600
H	4.40457600	-4.34515600	-4.43820000
C	3.63286100	-4.17548000	-0.62437600
H	3.42795900	-4.14011200	0.43964900
N	2.18614200	0.81794900	-0.70465300
S	3.75505400	1.15064900	-0.44080200
C	4.69908900	-0.39834200	-0.95709800
O	4.15511100	2.14889800	-1.43507200
O	4.08692100	1.32760700	0.97639200
F	5.93508400	-0.03965000	-1.31465700
F	4.09887400	-0.98116900	-2.00816900
F	4.77581200	-1.27048000	0.04578000
H	-0.46017900	0.27077300	-3.68979100

TS-1-2-3S

l imaginary frequencies

H = -4967.741922

G = -4967.924203

E(M06-2X-DCM) = -4968.522027

O	2.18805500	1.85249200	0.49925300
O	3.15711000	-0.16276100	-0.82287600
P	1.94715300	0.28210100	0.17058900
O	2.02644400	-0.40955500	1.52145000
N	0.56803600	0.18710800	-0.65919800
S	0.02067400	-1.10444700	-1.41688900
C	0.46185200	-0.82700100	-3.21478400
F	0.03034000	-1.86484000	-3.93375100

F	-0.12140800	0.28904800	-3.66916700
F	1.78411800	-0.71109700	-3.35560400
C	-0.65406900	-0.35798900	4.38602800
C	-1.04097800	-1.83508700	3.97593600
H	-0.58921700	-2.49087900	4.73186700
H	-2.12823600	-1.92018100	4.04225900
C	-0.60264100	-2.29470300	2.63300000
C	-1.05772900	0.66221300	3.25584900
H	-0.15969600	1.17642500	2.90661200
H	-1.73481000	1.41251000	3.66940300
N	-1.67127400	0.08461100	2.05665100
C	-3.04004700	-0.07745200	1.90605500
N	-3.36994700	-0.50617400	0.65211300
C	-4.62941500	-0.74024600	0.05798900
C	-5.77841900	-1.14104400	0.75249500
C	-4.68471200	-0.61050000	-1.33855700
C	-6.96331000	-1.36991100	0.05046800
C	-5.87794400	-0.83659900	-2.01876100
H	-3.79078800	-0.33530100	-1.88619400
C	-7.03228600	-1.21370100	-1.33251900
H	-7.95737400	-1.39697800	-1.86504500
C	-5.93046400	-0.58497200	-3.50146700
C	-8.20388000	-1.74650200	0.81870200
F	-6.15651800	0.72914000	-3.76999700
F	-6.92126900	-1.27864800	-4.10021000
F	-4.77305900	-0.90982000	-4.11380700
F	-7.91504200	-2.48582500	1.91170300
F	-9.06485500	-2.46215600	0.06046200
F	-8.87466500	-0.65338000	1.24875600
S	-4.11950100	0.19828700	3.16630200
H	-5.74862800	-1.27289700	1.82356700
C	0.70541300	-2.60894500	2.26182500
H	-2.60203600	-0.58400200	-0.02285000
H	1.42203300	-2.81001100	3.05971800
H	0.82326500	-3.20718300	1.35728100
O	-1.45796200	-1.05944000	-1.41883300
H	-1.14560600	0.24154200	1.19692300
O	0.65986400	-2.37515100	-1.04085900
H	1.17979400	-1.52680900	1.84619300
C	7.03061900	-0.02050000	0.77827800
C	6.42876400	1.12644500	0.27261400
C	5.16824800	1.06042700	-0.34136300
C	5.05958000	-1.33058400	0.14828800
C	6.35809500	-1.23779700	0.67954300

C	2. 25976400	2. 80237400	-0. 53134000
C	3. 44683300	2. 94153300	-1. 25111800
C	3. 46891300	3. 79430600	-2. 36714000
C	2. 36852900	4. 58266300	-2. 68258700
C	1. 23459700	4. 51274100	-1. 87670900
C	1. 14064100	3. 61460400	-0. 79896100
H	6. 82879200	-2. 14556600	1. 04482900
H	0. 37986700	5. 14694100	-2. 09051100
C	4. 85185300	2. 39395900	-1. 00804100
C	5. 68396100	3. 36016800	-0. 09804800
H	5. 91006000	4. 30917000	-0. 59342900
H	5. 10134300	3. 58422200	0. 80297700
H	4. 66644000	3. 60997900	-4. 17919900
H	5. 41281600	4. 58382900	-2. 91721300
C	4. 47203900	-0. 14531100	-0. 33325600
H	8. 01373700	0. 02389100	1. 24001800
H	2. 39042800	5. 25206200	-3. 53873100
C	6. 94215900	2. 54971300	0. 28177300
H	7. 74640400	2. 68889100	-0. 45401700
H	7. 35417300	2. 83958300	1. 25505600
C	4. 79175900	3. 69454100	-3. 09379400
C	5. 42069600	2. 43353700	-2. 46667000
H	6. 51469800	2. 43397600	-2. 48813000
H	5. 07597600	1. 54160100	-3. 00237000
C	-0. 11912800	3. 60750700	0. 00811500
C	-0. 10516200	4. 04993100	1. 35529200
C	-1. 34808000	3. 28313900	-0. 62105400
C	1. 09326700	4. 43068400	2. 04190800
C	-1. 35094100	4. 15971900	2. 08220600
C	-2. 58759100	3. 43421500	0. 10781000
C	1. 06952400	4. 84794300	3. 34733800
H	2. 03722300	4. 39259300	1. 51087800
C	-1. 33155900	4. 59623400	3. 44479800
C	-2. 55487300	3. 85864100	1. 43901600
C	-0. 15738200	4. 92594100	4. 06605900
H	1. 99644600	5. 12942900	3. 84001400
H	-2. 27908100	4. 66546700	3. 97388800
H	-3. 48902300	3. 95666800	1. 98739100
H	-0. 15655100	5. 25911800	5. 10037400
C	4. 38530400	-2. 66411200	0. 10380300
C	4. 09602600	-3. 27389400	-1. 14227000
C	4. 11966700	-3. 35512400	1. 31331200
C	4. 38590400	-2. 65341000	-2. 39921000
C	3. 50980700	-4. 59447700	-1. 17146900

C	3.56797300	-4.69110300	1.26584100
C	4.08758700	-3.26960900	-3.58591000
H	4.85593400	-1.67697900	-2.40749400
C	3.20886200	-5.20053200	-2.43085000
C	3.26920700	-5.26796000	0.02856300
C	3.48314000	-4.55822200	-3.60699500
H	4.31623600	-2.77163000	-4.52426500
H	2.75705700	-6.18950400	-2.43010400
H	2.84550700	-6.26978200	-0.00155200
H	3.24858900	-5.02795100	-4.55816500
C	-2.63451800	2.52067300	-2.55433200
H	-2.66182200	2.13470900	-3.56967900
C	-1.42752600	2.79057100	-1.96392400
H	-0.51108200	2.60290400	-2.50816300
C	-3.85533100	2.71504000	-1.84664900
H	-4.79826600	2.48676000	-2.33410300
C	-3.82637800	3.14602100	-0.54761100
H	-4.74691000	3.27180100	0.01684300
C	4.12539000	-3.49740900	3.75710600
H	4.32460500	-3.04046000	4.72302100
C	3.61552200	-4.82678400	3.70132500
H	3.44309300	-5.37826600	4.62174300
C	3.33645400	-5.39745300	2.48847100
H	2.93367300	-6.40598600	2.42962700
C	4.36101600	-2.78687200	2.60750100
H	4.72486500	-1.76847700	2.67151600
H	-1.37538000	-2.41815800	1.87770500
C	-1.42044400	-0.05098700	5.68944800
H	-1.17027600	0.95732900	6.03945400
H	-2.50124300	-0.09849500	5.53620800
H	-1.13974000	-0.75416000	6.48288500
C	0.85358200	-0.22949900	4.68001900
H	1.06836400	0.78594100	5.03431700
H	1.15874900	-0.92356400	5.47262600
H	1.47851100	-0.39750000	3.80076500

TS-1-2-3S-1

l imaginary frequencies

H = -4967.741923

G = -4967.924204

E(M06-2X-DCM) = -4968.522021

O	2.18825400	1.85237900	0.49969200
O	3.15710300	-0.16274300	-0.82280000
P	1.94716900	0.28206100	0.17071500

O	2.02636800	-0.40983900	1.52146200
N	0.56807700	0.18740300	-0.65913600
S	0.02051200	-1.10390800	-1.41712200
C	0.46184100	-0.82612200	-3.21494900
F	0.03045100	-1.86389100	-3.93412200
F	-0.12143300	0.28996100	-3.66924500
F	1.78410500	-0.71012300	-3.35560500
C	-0.65426100	-0.35895600	4.38620400
C	-1.04122500	-1.83590400	3.97571400
H	-0.58955600	-2.49192600	4.73150900
H	-2.12848800	-1.92097200	4.04195500
C	-0.60281800	-2.29524300	2.63270200
C	-1.05795200	0.66156200	3.25630200
H	-0.15996500	1.17600900	2.90729900
H	-1.73517400	1.41162000	3.67005400
N	-1.67137900	0.08424000	2.05691900
C	-3.04015300	-0.07783300	1.90619500
N	-3.36991100	-0.50650900	0.65220900
C	-4.62937900	-0.74025300	0.05793600
C	-5.77836400	-1.14141900	0.75224400
C	-4.68463100	-0.60987700	-1.33855500
C	-6.96323300	-1.37002000	0.05008800
C	-5.87782900	-0.83576200	-2.01889400
H	-3.79070400	-0.33437700	-1.88603300
C	-7.03217000	-1.21321500	-1.33283200
H	-7.95722600	-1.39635100	-1.86546400
C	-5.93038700	-0.58352200	-3.50149700
C	-8.20381800	-1.74700900	0.81810200
F	-6.15703700	0.73060300	-3.76948200
F	-6.92085400	-1.27739300	-4.10058300
F	-4.77281400	-0.90757100	-4.11392600
F	-7.91497100	-2.48655600	1.91095400
F	-9.06458900	-2.46262500	0.05959300
F	-8.87483800	-0.65411200	1.24834900
S	-4.11974800	0.19781000	3.16633600
H	-5.74858900	-1.27372000	1.82326300
C	0.70526600	-2.60933100	2.26144500
H	-2.60194300	-0.58429300	-0.02270600
H	1.42186200	-2.81059100	3.05931400
H	0.82310000	-3.20748000	1.35683900
O	-1.45811300	-1.05867800	-1.41909600
H	-1.14566900	0.24138700	1.19725700
O	0.65945500	-2.37478700	-1.04131400
H	1.17971300	-1.52714100	1.84602900

C	7.03057000	-0.02118100	0.77849500
C	6.42883800	1.12593300	0.27306800
C	5.16834100	1.06016200	-0.34097400
C	5.05944400	-1.33095100	0.14811500
C	6.35794400	-1.23840100	0.67944500
C	2.26004900	2.80242400	-0.53074400
C	3.44715300	2.94160900	-1.25045200
C	3.46936700	3.79458200	-2.36632200
C	2.36906800	4.58309500	-2.68166600
C	1.23509200	4.51312100	-1.87584700
C	1.14100500	3.61480100	-0.79826500
H	6.82855100	-2.14629700	1.04453100
H	0.38043200	5.14744300	-2.08957300
C	4.85210500	2.39386300	-1.00739200
C	5.68424600	3.35980400	-0.09715300
H	5.91045200	4.30889500	-0.59231300
H	5.10159700	3.58371200	0.80388800
H	4.66700200	3.61050300	-4.17834100
H	5.41336900	4.58404600	-2.91611200
C	4.47202000	-0.14551100	-0.33315500
H	8.01367000	0.02301400	1.24028800
H	2.39105700	5.25265400	-3.53768300
C	6.94235400	2.54915600	0.28256500
H	7.74665300	2.68842800	-0.45314700
H	7.35433600	2.83877900	1.25593600
C	4.79225100	3.69484100	-3.09291000
C	5.42104100	2.43366800	-2.46598400
H	6.51504300	2.43400800	-2.48738100
H	5.07626700	1.54186300	-3.00186700
C	-0.11881000	3.60763700	0.00873200
C	-0.10490900	4.04982300	1.35598300
C	-1.34773800	3.28344400	-0.62057500
C	1.09349600	4.43040900	2.04273600
C	-1.35072900	4.15953800	2.08284200
C	-2.58728100	3.43438300	0.10825600
C	1.06969200	4.84746600	3.34822800
H	2.03748200	4.39235600	1.51175500
C	-1.33141000	4.59585100	3.44550000
C	-2.55462900	3.85857700	1.43954100
C	-0.15725800	4.92541200	4.06688300
H	1.99659600	5.12883100	3.84100700
H	-2.27896300	4.66505700	3.97453900
H	-3.48880700	3.95651800	1.98788400
H	-0.15647600	5.25843200	5.10124900

C	4.38504500	-2.66440300	0.10325400
C	4.09574600	-3.27383100	-1.14298800
C	4.11929000	-3.35570100	1.31257300
C	4.38572000	-2.65304700	-2.39976100
C	3.50940000	-4.59435000	-1.17255100
C	3.56747200	-4.69161500	1.26473600
C	4.08737300	-3.26890500	-3.58663000
H	4.85585200	-1.67666300	-2.40777800
C	3.20843100	-5.20004600	-2.43210100
C	3.26869700	-5.26812300	0.02729600
C	3.48280000	-4.55745400	-3.60807000
H	4.31610000	-2.77070500	-4.52484900
H	2.75653000	-6.18897500	-2.43162500
H	2.84490600	-6.26989800	-0.00309300
H	3.24822700	-5.02690700	-4.55937100
C	-2.63408400	2.52138800	-2.55408400
H	-2.66133200	2.13562100	-3.56950400
C	-1.42712900	2.79119300	-1.96356100
H	-0.51066700	2.60370200	-2.50782900
C	-3.85492700	2.71559700	-1.84640900
H	-4.79786300	2.48744100	-2.33392700
C	-3.82603400	3.14631100	-0.54727800
H	-4.74659700	3.27199100	0.01714700
C	4.12488800	-3.49860800	3.75632900
H	4.32410100	-3.04192100	4.72236900
C	3.61490700	-4.82792300	3.70018700
H	3.44238800	-5.37962500	4.62045500
C	3.33583900	-5.39825700	2.48717400
H	2.93296600	-6.40673700	2.42805400
C	4.36063200	-2.78779800	2.60691600
H	4.72456000	-1.76944900	2.67120800
H	-1.37556300	-2.41870400	1.87741200
C	-1.42068200	-0.05224500	5.68967000
H	-1.17055800	0.95600400	6.03989600
H	-2.50147900	-0.09975000	5.53638300
H	-1.13999700	-0.75557500	6.48297400
C	0.85338200	-0.23056700	4.68024600
H	1.06817400	0.78478100	5.03480200
H	1.15853500	-0.92483200	5.47268400
H	1.47831900	-0.39836100	3.80095800

TS-1-2-3S-2

l imaginary frequencies

H = -4967.741359

G = -4967.923966

E(M06-2X-DCM) = -4968.520519

O	2.06917700	1.87186100	0.41529900
O	3.30786500	0.04223500	-0.93866900
P	1.89977000	0.37733300	-0.19454700
O	1.66129100	-0.48089600	1.04046900
N	0.86248700	0.41982200	-1.41658800
S	-0.28107000	-0.59158700	-1.80131600
C	0.58542200	-2.06528200	-2.56076200
F	-0.31721600	-2.96658400	-2.95371200
F	1.32069300	-1.68995500	-3.60376600
F	1.39012500	-2.63427700	-1.64195600
C	-0.51716200	-1.02330300	4.23188000
C	-0.91082100	-2.42485900	3.62172100
H	-0.39322500	-3.18041300	4.22809400
H	-1.98853300	-2.54951000	3.75601700
C	-0.58093000	-2.66902500	2.19124900
C	-1.03460700	0.15004700	3.31651200
H	-0.18119600	0.74657700	2.98563800
H	-1.69702200	0.79810400	3.89290500
N	-1.73326600	-0.25537400	2.10291200
C	-3.10006800	-0.36681600	1.98134800
N	-3.46988000	-0.63880500	0.68976100
C	-4.73067900	-0.76073000	0.07388500
C	-5.92185500	-1.08464900	0.73688900
C	-4.74819800	-0.58602100	-1.32121600
C	-7.10544300	-1.20631300	0.00608800
C	-5.93990700	-0.71064700	-2.02899300
H	-3.83020600	-0.34502100	-1.84946000
C	-7.13298700	-1.01904300	-1.37367000
H	-8.05686200	-1.12459200	-1.92883300
C	-5.95418100	-0.43137800	-3.50852400
C	-8.38656600	-1.50091900	0.74337200
F	-6.17292100	0.88664800	-3.76008800
F	-6.93654600	-1.11148700	-4.13909000
F	-4.78740000	-0.75338700	-4.09946300
F	-8.18104000	-2.30244600	1.81082900
F	-9.29494000	-2.10953300	-0.05215200
F	-8.96529300	-0.36926700	1.20650200
S	-4.13641600	-0.20881100	3.29914900
H	-5.92202300	-1.24013100	1.80551800
C	0.68903800	-2.86246000	1.65845100
H	-2.69586000	-0.69519500	0.02455300
H	1.50579700	-3.09307700	2.34180800

H	0.73958100	-3.34113600	0.68004900
O	-1.13987100	-0.06524900	-2.85892000
H	-1.20488600	-0.18534000	1.23683600
O	-0.96374200	-1.19425700	-0.61449200
H	1.02144300	-1.68302300	1.28599100
C	6.98045400	0.37229200	1.05787100
C	6.34552300	1.50183700	0.55434900
C	5.14887100	1.39295100	-0.17355400
C	5.17294000	-1.02530800	0.18372000
C	6.40664700	-0.87852700	0.84120100
C	2.16589800	2.97347900	-0.44846900
C	3.38095200	3.24041400	-1.07272300
C	3.42562700	4.21025800	-2.08630000
C	2.31135700	4.99535600	-2.36217900
C	1.14849200	4.80907100	-1.61482100
C	1.03559800	3.78623500	-0.65704000
H	6.90660700	-1.77255600	1.20145500
H	0.28789600	5.44803300	-1.78728400
C	4.79509900	2.74789900	-0.78239700
C	5.49327400	3.70115800	0.24876500
H	5.69087100	4.69287800	-0.16826800
H	4.83100700	3.82907900	1.11284800
H	4.71833000	4.22154900	-3.84117000
H	5.35860800	5.12248400	-2.47212800
C	4.54212400	0.14263700	-0.28958900
H	7.91487600	0.45772400	1.60661600
H	2.34489200	5.75683600	-3.13718000
C	6.76807900	2.94823500	0.67802800
H	7.61197800	3.17419100	0.01129000
H	7.09214200	3.20505200	1.69294700
C	4.78756500	4.22499300	-2.74745500
C	5.44759200	2.94248500	-2.19149200
H	6.53932700	3.00189600	-2.14278500
H	5.18621100	2.08567200	-2.82294900
C	-0.23449500	3.63893800	0.11946900
C	-0.23461000	3.86833200	1.52018500
C	-1.45239100	3.36993200	-0.55675500
C	0.94581400	4.20048000	2.26140900
C	-1.47882700	3.80102500	2.25429800
C	-2.69218300	3.33935800	0.18888000
C	0.90848200	4.41093300	3.61545100
H	1.88715500	4.29876600	1.73340500
C	-1.47419400	4.02020200	3.66833900
C	-2.67020400	3.54333000	1.57100400

C	-0.31549700	4.31146300	4.33605900
H	1.82240600	4.66443600	4.14636300
H	-2.42119500	3.95598100	4.19887600
H	-3.60327300	3.50087800	2.12839600
H	-0.32580600	4.48082800	5.40941900
C	4.61873100	-2.40215900	-0.00154400
C	4.50744900	-2.95814800	-1.30057900
C	4.30121400	-3.18712900	1.13635400
C	4.84849900	-2.23558400	-2.48863100
C	4.05009200	-4.32064300	-1.45795600
C	3.88233000	-4.56067500	0.96402800
C	4.70718300	-2.79579900	-3.73086200
H	5.22654300	-1.22422700	-2.39846200
C	3.91614500	-4.86796200	-2.77238000
C	3.76004300	-5.08548800	-0.32535500
C	4.22660200	-4.12771700	-3.88026400
H	4.96724100	-2.21992900	-4.61470000
H	3.56196500	-5.89147300	-2.86935500
H	3.43649300	-6.11691900	-0.45028500
H	4.11773900	-4.55268800	-4.87417900
C	-2.72038400	2.87163500	-2.58553000
H	-2.73714000	2.65065600	-3.64852500
C	-1.52211500	3.10466900	-1.96255600
H	-0.60412400	3.05374700	-2.53451400
C	-3.94042900	2.87560500	-1.85251600
H	-4.87461800	2.66941300	-2.36580500
C	-3.92056700	3.09323800	-0.50090400
H	-4.83981300	3.07487100	0.07934000
C	4.08117200	-3.47600900	3.55744600
H	4.14373600	-3.06316000	4.56081000
C	3.70179100	-4.83799700	3.38112600
H	3.49060400	-5.45649100	4.24927700
C	3.59750300	-5.35674900	2.11829200
H	3.29697100	-6.39087900	1.96676100
C	4.36329900	-2.68009800	2.47615400
H	4.63322500	-1.64211400	2.63051500
H	-1.41415800	-2.71438700	1.49493000
C	-1.18449000	-0.94807700	5.62047400
H	-0.92407300	-0.00219100	6.10967000
H	-2.27385300	-0.99686500	5.53826000
H	-0.83848300	-1.76159100	6.26970100
C	1.00695300	-0.89514800	4.41518100
H	1.23629000	0.05661300	4.90935500
H	1.39733400	-1.69874700	5.05132900

H 1.54962100 -0.90164100 3.46699300

TS-1-2-3R

1 imaginary frequencies

H = -4967.742916

G = -4967.925010

E(M06-2X-DCM) = -4968.520385

O	1.74434700	-1.80242700	-0.45795100
O	3.49991000	-0.02940700	0.23494100
P	1.90731100	-0.28495100	0.07846100
O	1.31556200	-0.07623400	1.47520700
N	1.37356900	0.66740500	-1.09801400
S	-0.17073600	0.87713900	-1.39396000
C	-0.29758300	0.43957900	-3.20468700
F	-1.57827800	0.52735300	-3.57766700
F	0.13593800	-0.80511100	-3.40845700
F	0.43127600	1.28333400	-3.94385000
C	-0.64483900	1.63798400	4.51646300
C	-0.74970900	2.90781400	3.59631300
H	-0.17393500	3.70256700	4.09200300
H	-1.79927200	3.20990800	3.56489700
C	-0.24083800	2.77804600	2.20440800
C	-1.34861600	0.40794000	3.83698700
H	-0.65370600	-0.43420700	3.81937500
H	-2.21781800	0.11537700	4.42789200
N	-1.78717600	0.59612600	2.45243500
C	-3.10521700	0.86388700	2.11650600
N	-3.34192000	0.65532000	0.78840000
C	-4.51726000	0.67829100	0.01419600
C	-5.73790700	1.25758800	0.38889700
C	-4.41426600	0.06020200	-1.24485600
C	-6.82624500	1.19160100	-0.48383900
C	-5.51500700	-0.00423000	-2.09231900
H	-3.47092900	-0.37736200	-1.55309700
C	-6.73652300	0.55909900	-1.72237400
H	-7.59408500	0.50576000	-2.38142000
C	-5.38930900	-0.76993500	-3.38188100
C	-8.11068500	1.87969700	-0.09725500
F	-4.18107900	-0.59861200	-3.95921800
F	-5.53242100	-2.10829700	-3.17694300
F	-6.32874300	-0.41251900	-4.28167600
F	-9.18477400	1.29929700	-0.67938800
F	-8.31307400	1.86284300	1.23647300
F	-8.11157400	3.17812800	-0.48018100

S	-4. 21932000	1. 41040300	3. 25438700
H	-5. 83699400	1. 73785500	1. 35105300
C	1. 08402200	2. 57377300	1. 83199900
H	-2. 52991200	0. 35097900	0. 24234900
H	1. 86595800	2. 73983500	2. 57241100
H	1. 34128500	2. 84049800	0. 80511800
O	-1. 04825800	-0. 12698000	-0. 72430000
H	-1. 25021000	0. 06676800	1. 76844100
O	-0. 58736700	2. 28155100	-1. 28699600
H	1. 10564800	1. 29167600	1. 70385200
C	5. 69884900	0. 04036700	-3. 32580000
C	5. 35684100	-1. 17078300	-2. 73423600
C	4. 71221100	-1. 20257900	-1. 48668200
C	4. 67818400	1. 24277400	-1. 45622300
C	5. 39437200	1. 23050500	-2. 66430700
C	2. 29264700	-2. 91639300	0. 18626400
C	3. 64384400	-3. 20486100	0. 00331600
C	4. 21412400	-4. 25964700	0. 73436600
C	3. 42264600	-5. 08569300	1. 52506600
C	2. 05138600	-4. 84625300	1. 59674300
C	1. 45334200	-3. 74790900	0. 95362800
H	5. 69004400	2. 18139500	-3. 09733300
H	1. 41825100	-5. 50738500	2. 18036400
C	4. 68142800	-2. 63668800	-0. 96393700
C	4. 67905000	-3. 42009600	-2. 32039400
H	3. 65423800	-3. 45082800	-2. 70783000
H	5. 02410100	-4. 45228900	-2. 20745200
H	5. 98379200	-5. 16381400	-0. 13431100
H	6. 26689100	-4. 44323700	1. 44617200
C	4. 30629500	-0. 00137700	-0. 91293600
H	6. 20559500	0. 06546000	-4. 28713300
H	3. 86068400	-5. 91603000	2. 07310900
C	5. 56773600	-2. 57454500	-3. 25887000
H	5. 28217500	-2. 67314600	-4. 31223900
H	6. 62285300	-2. 87369100	-3. 18992700
C	5. 70911500	-4. 31795400	0. 51111900
C	5. 99573200	-2. 96686200	-0. 17710400
H	6. 15636900	-2. 19127000	0. 58071400
H	6. 87655300	-2. 98628500	-0. 82573900
C	-0. 01948300	-3. 52678100	1. 08768800
C	-0. 58666100	-3. 35100600	2. 37720600
C	-0. 85714900	-3. 56961000	-0. 05657900
C	0. 19634300	-3. 27097100	3. 57646200
C	-2. 02211800	-3. 24042400	2. 51693100

C	-2.28356400	-3.38984900	0.09524100
C	-0.39193100	-3.16892100	4.81172900
H	1.27698000	-3.29112200	3.49975000
C	-2.59542800	-3.13193500	3.82344900
C	-2.82688200	-3.24291900	1.37405300
C	-1.80875700	-3.11443400	4.94354600
H	0.23069400	-3.12261700	5.70160300
H	-3.67747500	-3.06414100	3.90439600
H	-3.90399300	-3.13605100	1.48405300
H	-2.25793200	-3.04230600	5.93026700
C	4.37964700	2.54600300	-0.78387000
C	3.53802900	3.49605100	-1.41457100
C	5.00903900	2.85793500	0.44859800
C	2.84553400	3.23061300	-2.64020500
C	3.33534600	4.78973400	-0.79951700
C	4.77390500	4.14490400	1.06431200
C	2.04541000	4.17588700	-3.22562100
H	2.93248400	2.24907600	-3.08832100
C	2.50068100	5.75186200	-1.45087600
C	3.95123400	5.07468900	0.42194000
C	1.87760000	5.45946200	-2.63301000
H	1.51435900	3.93655900	-4.14216500
H	2.36979000	6.72247700	-0.97810300
H	3.79139700	6.04807700	0.88191200
H	1.24107500	6.19592000	-3.11562000
C	-1.19695700	-3.79636800	-2.46727000
H	-0.78893100	-3.96918600	-3.45940700
C	-0.36386500	-3.80660200	-1.37957600
H	0.69304300	-3.99936700	-1.52043400
C	-2.59285500	-3.56199800	-2.31654400
H	-3.23824100	-3.52923000	-3.18879100
C	-3.11858000	-3.37949000	-1.06644100
H	-4.18526400	-3.21636800	-0.93753900
C	6.49167200	2.29378100	2.31096200
H	7.16683300	1.59196500	2.79325600
C	6.23422200	3.55219300	2.92500300
H	6.70824700	3.79769200	3.87146300
C	5.40257900	4.45010000	2.31256200
H	5.20863200	5.42206200	2.76056700
C	5.90385300	1.96190300	1.11823300
H	6.12489300	1.00367900	0.66233400
C	-1.36556700	1.98705700	5.83470600
H	-0.88204900	2.83275900	6.33842600
H	-2.41564200	2.23535700	5.65450200

H	-1.33248600	1.13210800	6.52026200
C	0.81804100	1.27536700	4.84291200
H	1.35518600	2.12746000	5.27702700
H	0.83597500	0.46572100	5.58208700
H	1.37097900	0.91780500	3.97046500
H	-0.96212800	2.86754800	1.39407900

INT-9

0 imaginary frequencies

H = -4333.090486

G = -4333.270521

E(M06-2X-DCM) = -4333.893400

C	0.00049200	-3.35021800	3.79353800
C	0.31241700	-2.21523600	4.82514200
H	-0.55409100	-2.15882800	5.49503800
H	1.14989100	-2.56063300	5.44149400
C	2.01354000	-0.44282600	3.98047600
C	3.09872100	-0.91333000	4.74011900
C	2.28926200	0.42542000	2.90950000
C	4.40529100	-0.52462300	4.44593600
H	2.92767100	-1.56883300	5.58842200
C	3.59452800	0.80687700	2.60835300
H	1.47310200	0.77710800	2.28588200
C	4.65981200	0.33404500	3.37730000
H	5.22525800	-0.90031000	5.05207200
H	3.77783100	1.46757800	1.76646600
H	5.67939100	0.62285800	3.13733100
C	0.60965000	-0.81186600	4.32185200
C	1.15703600	-3.62806400	2.80049600
H	1.00183300	-4.61917900	2.35106500
H	2.10912800	-3.67798800	3.33803200
N	1.28667400	-2.64249400	1.73743100
C	2.32516700	-2.60949400	0.86287100
N	2.14035500	-1.63517500	-0.09985400
C	2.93865300	-1.13676400	-1.13137500
C	4.18353700	-1.64518700	-1.53480500
C	2.41154900	-0.02177800	-1.81575900
C	4.86748000	-1.03784600	-2.59060800
C	3.10998200	0.56366700	-2.86444100
H	1.45636900	0.39192500	-1.50903900
C	4.35104300	0.06449200	-3.26736800
H	4.89791200	0.52248800	-4.08249100
C	2.50521700	1.72024900	-3.60973500
C	6.23424700	-1.55610000	-2.95962300

F	1. 87686300	1. 32555100	-4. 74585100
F	3. 43517700	2. 62965800	-3. 97757500
F	1. 57755200	2. 38043100	-2. 86885400
F	6. 54476900	-1. 28022000	-4. 24804400
F	6. 33118000	-2. 89145300	-2. 79740000
F	7. 20079400	-0. 99405900	-2. 19631900
S	3. 63971400	-3. 65875600	0. 97963300
C	-0. 16456700	-4. 64777200	4. 61646900
H	-0. 91943600	-4. 51917000	5. 40078900
H	-0. 48328900	-5. 47798100	3. 97623800
H	0. 77675300	-4. 93744200	5. 09938600
C	-1. 32762600	-3. 06915500	3. 06772800
H	-1. 54486100	-3. 84828900	2. 33033900
H	-2. 15512600	-3. 04941900	3. 78766600
H	-1. 33345500	-2. 10669800	2. 54725800
H	4. 60062300	-2. 50223000	-1. 02490100
C	-0. 37167700	0. 11235400	4. 26817500
H	1. 25230200	-1. 14090000	-0. 02259400
H	-1. 38552100	-0. 12843500	4. 58209300
H	-0. 16396300	1. 15213500	4. 02977200
H	0. 46998400	-2. 08299200	1. 51479400
H	-1. 69310000	0. 60281500	2. 37045100
O	-0. 95675500	1. 73893900	-0. 41250500
O	-2. 92151000	0. 06216500	-0. 62617200
P	-1. 59824700	0. 39876400	0. 23018200
O	-0. 54131500	-0. 64134300	0. 30439200
C	-3. 38650700	5. 13315400	-0. 82538100
C	-3. 44796700	4. 10543600	-1. 76020400
C	-2. 58497700	3. 00183700	-1. 67076500
C	-1. 60981400	3. 94240000	0. 36241700
C	-2. 44990500	5. 05776300	0. 20456900
C	-2. 71278600	-0. 34469300	-1. 96430400
C	-2. 49610100	0. 62822100	-2. 93649800
C	-2. 09069300	0. 22834500	-4. 21932800
C	-2. 03058300	-1. 12100700	-4. 55171000
C	-2. 38221100	-2. 07269500	-3. 59540100
C	-2. 71302800	-1. 71604600	-2. 27584700
H	-2. 36598200	5. 86895100	0. 92154200
H	-2. 37931900	-3. 12680400	-3. 85517800
C	-2. 72124800	2. 13488700	-2. 91618400
C	-4. 19062300	2. 48009000	-3. 33715900
H	-4. 37546600	2. 27908800	-4. 39670600
H	-4. 88177500	1. 86073200	-2. 75368900
H	-0. 78803500	1. 31807000	-5. 57840100

H	-2.50874900	1.59486600	-5.85227100
C	-1.73098100	2.90244100	-0.57589000
H	-4.05001900	5.99103700	-0.89782500
H	-1.72475100	-1.43524200	-5.54618500
C	-4.37005400	3.96361800	-2.95107100
H	-4.06460000	4.63057300	-3.76918800
H	-5.40894100	4.21597000	-2.71062900
C	-1.75266200	1.43194600	-5.07193900
C	-1.73122300	2.58416700	-4.04225800
H	-2.00419800	3.55346100	-4.47071800
H	-0.72646700	2.67519300	-3.61998600
C	-3.09258900	-2.78957200	-1.30592000
C	-4.42717000	-2.86760300	-0.83199200
C	-2.15166400	-3.79033300	-0.95740600
C	-5.43809300	-1.91351500	-1.17673000
C	-4.81848000	-3.97266300	0.01388100
C	-2.56974200	-4.90890200	-0.14160000
C	-6.71755700	-2.02040900	-0.69745600
H	-5.18402100	-1.09394200	-1.83897300
C	-6.16242200	-4.04436700	0.49745600
C	-3.88540700	-4.96520900	0.32516500
C	-7.08806300	-3.09518400	0.15920100
H	-7.46154500	-1.27928300	-0.97716100
H	-6.43273600	-4.87970100	1.13917400
H	-4.19296500	-5.80603900	0.94384500
H	-8.10648800	-3.16154400	0.53198400
C	-0.60665200	3.94516400	1.47298400
C	0.76922200	4.11153200	1.17294300
C	-1.04355300	3.90119800	2.81958800
C	1.27486900	4.16122100	-0.16577700
C	1.72040100	4.25518100	2.25196000
C	-0.07980700	4.05119200	3.88793100
C	2.61208400	4.32106800	-0.42036700
H	0.58454000	4.06372300	-0.99461200
C	3.10561300	4.43427400	1.94402100
C	1.27104300	4.22620100	3.57515600
C	3.54344300	4.46436500	0.64713400
H	2.96519000	4.32956500	-1.44737700
H	3.80497000	4.54158500	2.76942900
H	1.99177300	4.33947300	4.38206500
H	4.59887900	4.59771200	0.42630000
C	0.09988200	-4.74389900	-1.03000000
H	1.13947300	-4.67745400	-1.33644100
C	-0.77903100	-3.74724100	-1.36695700

H	-0.43019500	-2.89618200	-1.93971100
C	-0.32803800	-5.86100500	-0.25660700
H	0.38347100	-6.64298800	-0.00709100
C	-1.62436800	-5.93478900	0.17723100
H	-1.96287100	-6.77619700	0.77764600
C	-2.80316000	3.66333500	4.50068600
H	-3.84876800	3.50237100	4.74915400
C	-1.85220200	3.83142900	5.54787500
H	-2.18067200	3.80505300	6.58315000
C	-0.53021300	4.01591800	5.24565100
H	0.20837900	4.13485600	6.03465300
C	-2.41468600	3.69723800	3.18635100
H	-3.14956200	3.55337100	2.40292400
O	-2.29016800	0.78364800	1.61442000

INT-9'

0 imaginary frequencies

H = -4333.080397

G = -4333.257910

E(M06-2X-DCM) = -4333.881586

O	-0.29282000	-2.77302700	0.13750400
O	-2.45691200	-1.37909300	-0.11867600
P	-0.82473000	-1.20314400	0.11693500
O	-0.33854900	-0.54077900	-1.16759400
C	-1.01198000	-5.11662700	-3.25453900
C	-1.97409500	-4.99401900	-2.25698400
C	-1.70491700	-4.26528700	-1.08949500
C	0.49922200	-3.69127400	-1.96041400
C	0.22180000	-4.48803200	-3.08423700
C	-3.16438600	-1.99536300	0.90527700
C	-3.23763000	-3.38852400	0.94616200
C	-3.80797600	-4.01482800	2.06492100
C	-4.38987600	-3.26455700	3.08140500
C	-4.40050600	-1.87370100	2.97363500
C	-3.78300200	-1.21219600	1.90008300
H	0.98905300	-4.59052700	-3.84656800
H	-4.87529700	-1.27440200	3.74542100
C	-2.84421900	-4.43830000	-0.09025800
C	-4.02668100	-4.74237200	-1.07183500
H	-4.41647600	-3.79253200	-1.45582900
H	-4.85231500	-5.26892500	-0.58251600
H	-4.60155700	-6.00235100	1.70519300
H	-3.32314600	-5.96532500	2.91526700
C	-0.50047300	-3.57187400	-0.97191000

H	-1.21263100	-5.69113300	-4.15555800
H	-4.83306300	-3.74916600	3.94787200
C	-3.38383200	-5.54395900	-2.22501000
H	-3.90943200	-5.41105400	-3.17779300
H	-3.38645800	-6.62251800	-2.01238400
C	-3.65121100	-5.51733500	1.97022500
C	-2.60704200	-5.67275500	0.84313100
H	-1.59734900	-5.60462700	1.26384900
H	-2.68303700	-6.62410300	0.30665200
C	-3.84795300	0.28272300	1.83448100
C	-3.13297500	1.07195400	2.76734600
C	-4.70955900	0.90104700	0.89398300
C	-2.20623500	0.50940300	3.70406100
C	-3.31471500	2.50657000	2.77921100
C	-4.86564300	2.33821400	0.90211800
C	-1.53338200	1.29757400	4.60014300
H	-2.00926100	-0.55382500	3.66318300
C	-2.60422700	3.29217800	3.74214400
C	-4.17487100	3.09962600	1.85007100
C	-1.74207900	2.70663500	4.63030500
H	-0.81456900	0.84857900	5.27930000
H	-2.76736700	4.36764800	3.75029900
H	-4.31197800	4.17933600	1.86596800
H	-1.20849000	3.31362100	5.35747000
C	1.82889700	-3.01231900	-1.85267100
C	2.19427900	-2.01904700	-2.79664900
C	2.75066400	-3.40467800	-0.84961400
C	1.29850000	-1.54430900	-3.80982400
C	3.51343000	-1.42843800	-2.74377400
C	4.05039000	-2.77502600	-0.78299800
C	1.68794400	-0.59955900	-4.72452700
H	0.28955200	-1.93690900	-3.83435200
C	3.88107600	-0.44725900	-3.71908000
C	4.40164100	-1.81512600	-1.73625500
C	3.00068100	-0.04643900	-4.68802500
H	0.98909700	-0.26896800	-5.48920800
H	4.88618400	-0.03262600	-3.67697600
H	5.38532900	-1.35359800	-1.68384400
H	3.29727700	0.69192700	-5.42863400
C	-6.29498900	0.78391300	-0.96489600
H	-6.85727600	0.19349800	-1.68358100
C	-5.46721300	0.15897700	-0.06887700
H	-5.38020600	-0.92137300	-0.07980800
C	-6.43344600	2.20141800	-0.96099400

H	-7.09874100	2.68021900	-1.67492800
C	-5.73992400	2.95214300	-0.04965400
H	-5.84333600	4.03472300	-0.02828000
C	3.36791200	-4.77244400	1.07908700
H	3.11966500	-5.54934400	1.79711800
C	4.63204200	-4.12190800	1.16105500
H	5.33119400	-4.40159300	1.94459200
C	4.96215200	-3.15353300	0.25239800
H	5.92075200	-2.64298900	0.30225600
C	2.46197700	-4.42613900	0.11142200
H	1.50457200	-4.93147000	0.06497200
C	-1.68889600	2.76594200	-3.39065100
C	-2.49251400	3.42314200	-2.22322700
H	-3.55520500	3.29479100	-2.45591100
H	-2.31583100	2.83544200	-1.31608200
C	-1.17076700	5.29569600	-0.97659700
C	-0.32082800	6.38710400	-1.24394800
C	-1.03527600	4.64344000	0.26278700
C	0.60700900	6.82782600	-0.29706600
H	-0.39622900	6.89290300	-2.20291700
C	-0.11195500	5.08712000	1.21025200
H	-1.68250000	3.80849700	0.51137700
C	0.71122300	6.18218900	0.93679000
H	1.24779200	7.67546100	-0.52651300
H	-0.04796000	4.57501700	2.16624900
H	1.43075400	6.52479800	1.67516800
C	-2.23072600	4.89694400	-1.94992900
C	-0.16298800	2.79970800	-3.14188900
H	0.16250800	3.83520900	-3.02875100
H	0.35263100	2.38653000	-4.02003000
N	0.24627700	2.02400800	-1.96684500
C	1.38227100	2.11763800	-1.28128100
N	1.75581800	1.06444800	-0.55576100
C	2.77441700	0.97852900	0.43732500
C	4.11582800	1.15451800	0.09962400
C	2.40216700	0.62219700	1.73800600
C	5.09550200	1.00129600	1.08177300
C	3.39550100	0.48425000	2.70799400
H	1.35388400	0.43350600	1.96328000
C	4.74133900	0.67374300	2.38959300
H	5.50405000	0.56462600	3.15084900
C	3.00408300	0.07983500	4.10870500
C	6.54360600	1.09733900	0.68484300
F	1.84970200	0.66673000	4.48950000

F	3.95296100	0.42930800	5.00868000
F	2.83009400	-1.25246700	4.21234300
F	6.97768400	-0.05995000	0.11732400
F	7.34692800	1.34314700	1.73818400
F	6.74925800	2.07177300	-0.22798700
S	2.41302000	3.55888200	-1.28433900
H	4.39663900	1.37399600	-0.92431600
H	1.09865800	0.25432300	-0.65276400
H	-0.23450700	1.11719900	-1.80950200
C	-2.97293100	5.84664800	-2.54232400
H	-3.76773600	5.59283700	-3.23855400
H	1.40722300	4.43582200	-1.49429800
H	-2.83142900	6.90294000	-2.33155500
C	-2.18425300	1.31227100	-3.55098100
H	-3.23516400	1.30992700	-3.86090400
H	-1.60739800	0.78495800	-4.32066100
H	-2.11928200	0.72907200	-2.62675400
C	-1.92889300	3.51285100	-4.71691600
H	-1.41629200	3.00864900	-5.54488200
H	-2.99834000	3.53310500	-4.95444200
H	-1.57802300	4.54900400	-4.67631700
O	-0.47841000	-0.61360800	1.44028700

TS-EF-1S'

l imaginary frequencies

H = -4333.064446

G = -4333.238914

E(M06-2X-DCM) = -4333.863838

O	0.57996300	2.50407500	0.39855000
O	2.61980400	1.10981200	-0.39729800
P	1.01524100	0.94808700	0.02085000
O	0.34572000	0.55431000	-1.28646600
C	0.70904400	5.28089400	-2.73822900
C	1.85589000	4.96876200	-2.01622800
C	1.79117600	4.10968900	-0.90948200
C	-0.59273000	3.79430000	-1.29061200
C	-0.50568400	4.72143500	-2.34429900
C	3.51105400	1.60577900	0.54213500
C	3.65416700	2.98865100	0.68696000
C	4.46197400	3.49984000	1.71428000
C	5.20328500	2.65088700	2.52816000
C	5.12856700	1.27777800	2.30796800
C	4.28131900	0.72602000	1.33090300
H	-1.41665200	4.98400300	-2.87432000

H	5. 72166800	0. 60052800	2. 91563100
C	3. 11875000	4. 13639900	-0. 16276000
C	4. 09171400	4. 48744300	-1. 33749100
H	4. 33007000	3. 56647700	-1. 88216000
H	5. 03337200	4. 92205100	-0. 98692500
H	5. 27156700	5. 47994200	1. 35930400
H	4. 25649500	5. 38399300	2. 79478500
C	0. 59351100	3. 46324400	-0. 60219400
H	0. 75012600	5. 95725100	-3. 58856300
H	5. 83489300	3. 04611900	3. 31986000
C	3. 27762400	5. 43546000	-2. 24575600
H	3. 57511700	5. 37099400	-3. 29901400
H	3. 40736200	6. 48539800	-1. 94733900
C	4. 36774600	5. 00844400	1. 77100000
C	3. 13331700	5. 29479000	0. 89201300
H	2. 22382200	5. 22505700	1. 49965900
H	3. 14834300	6. 28504100	0. 42598600
C	4. 29290700	-0. 76181900	1. 16945100
C	3. 85570400	-1. 58430800	2. 23694700
C	4. 89293800	-1. 34720600	0. 02649300
C	3. 21128100	-1. 05501300	3. 40244100
C	4. 06481100	-3. 01331400	2. 17581000
C	5. 05321500	-2. 78318300	-0. 04251300
C	2. 86314600	-1. 86503900	4. 45182800
H	2. 97961000	0. 00233500	3. 43284200
C	3. 69028200	-3. 82192500	3. 29468700
C	4. 64413100	-3. 57476800	1. 03477600
C	3. 12065700	-3. 26561500	4. 40783200
H	2. 37503400	-1. 43778600	5. 32365900
H	3. 87186600	-4. 89282700	3. 23923600
H	4. 79981200	-4. 65126000	0. 99268800
H	2. 84914400	-3. 88976100	5. 25536500
C	-1. 93562700	3. 23879400	-0. 93656400
C	-2. 66529100	2. 49334100	-1. 89755100
C	-2. 52815500	3. 54856900	0. 31454000
C	-2. 10988900	2. 09882500	-3. 15949500
C	-4. 02200800	2. 08471200	-1. 61011600
C	-3. 86948800	3. 09289700	0. 60423100
C	-2. 84981200	1. 40081400	-4. 07870200
H	-1. 07653900	2. 34594100	-3. 37081200
C	-4. 76187800	1. 36193500	-2. 59948900
C	-4. 58414600	2. 38680900	-0. 36725800
C	-4. 19905000	1. 03426400	-3. 80372000
H	-2. 40248400	1. 11640700	-5. 02788100

H	-5.78168000	1.06840500	-2.36135900
H	-5.59398100	2.04813400	-0.14615000
H	-4.77162500	0.48645300	-4.54752400
C	6.00032900	-1.16271800	-2.14717400
H	6.38251700	-0.54662800	-2.95676500
C	5.40178500	-0.57142800	-1.06480100
H	5.31487600	0.50787600	-1.02147400
C	6.13385300	-2.57936800	-2.22068000
H	6.61625300	-3.03149700	-3.08353700
C	5.67194600	-3.36199900	-1.19597900
H	5.78761200	-4.44341800	-1.22846100
C	-2.45962500	4.59476900	2.52289300
H	-1.92820700	5.18230700	3.26675100
C	-3.76715400	4.11345600	2.81481400
H	-4.21867600	4.33022000	3.77912000
C	-4.45084800	3.38948300	1.87684700
H	-5.45612800	3.02694500	2.07854000
C	-1.86524300	4.32543800	1.31822900
H	-0.87193500	4.70632800	1.11414900
C	1.45599100	-2.81340300	-3.63207500
C	1.64008300	-3.49491400	-2.23387600
H	2.52701100	-4.14618700	-2.30338200
H	1.93527900	-2.73120500	-1.51200100
C	0.39968700	-4.31660700	-0.15046400
C	0.56253500	-3.11947600	0.58110100
C	-0.00509400	-5.47747300	0.54987300
C	0.28934600	-3.07414200	1.94463700
H	0.83941700	-2.19084600	0.09686600
C	-0.24214800	-5.43588800	1.91779900
H	-0.08974600	-6.42280300	0.02270400
C	-0.10881700	-4.23086100	2.61612000
H	0.39637400	-2.12726700	2.46192600
H	-0.53219700	-6.34242000	2.44161300
H	-0.31123100	-4.19488300	3.68270200
C	0.56435300	-4.34821500	-1.60683900
C	0.00989300	-2.29254300	-3.86501300
H	-0.67099500	-3.09273000	-4.15246500
H	0.03723400	-1.58249300	-4.70290700
N	-0.53861500	-1.61511700	-2.70245800
C	-1.70237600	-1.84675200	-2.07666000
N	-1.98999800	-0.96757200	-1.09580400
C	-2.97856600	-1.03276200	-0.08465600
C	-4.32320700	-1.28245000	-0.36517300
C	-2.57266700	-0.75032200	1.22507300

C	-5.25487300	-1.26281700	0.67208800
C	-3.51660500	-0.75449200	2.25212900
H	-1.52700300	-0.53042500	1.43165800
C	-4.86151700	-1.00987900	1.98623100
H	-5.59023200	-1.00792600	2.78701500
C	-3.06252800	-0.44553800	3.65590400
C	-6.71195000	-1.40567100	0.32811700
F	-1.91377000	-1.09471000	3.95795500
F	-3.98492400	-0.81479800	4.57476700
F	-2.83062500	0.87053600	3.82987900
F	-7.20985000	-0.24431700	-0.17897300
F	-7.46571300	-1.71823400	1.40207000
F	-6.92115400	-2.35292600	-0.61040800
S	-2.72563300	-3.20158200	-2.46562100
H	-4.64506200	-1.44955300	-1.38429800
H	-1.26292000	-0.23934600	-0.96895800
H	-0.00992000	-0.80409500	-2.33491900
C	-0.33247000	-5.10700500	-2.36499800
H	-0.09761400	-5.32589900	-3.40332900
H	-1.36803400	-4.24819600	-2.46348000
H	-0.89895200	-5.88698500	-1.85671000
C	2.43612600	-1.61813000	-3.66292600
H	3.46078400	-1.95184800	-3.46941700
H	2.41892800	-1.13463400	-4.64718600
H	2.19324800	-0.86185000	-2.90791700
C	1.81749100	-3.75538800	-4.79890100
H	1.69528100	-3.23977300	-5.75900100
H	2.86445400	-4.07039400	-4.72663400
H	1.19817800	-4.65761900	-4.83205100
O	0.82565400	0.12284000	1.25052500

TS-EF-1S'-1

l imaginary frequencies

H = -4333.066311

G = -4333.238693

E(M06-2X-DCM) = -4333.856208

O	-2.81488900	1.14219200	-0.00930100
O	-0.61427000	1.98821700	-1.08335500
P	-1.17596800	0.96599100	0.10129600
O	-0.73039700	-0.41129600	-0.33025600
C	-4.62619700	0.15288500	-3.66326000
C	-4.04514400	1.40112600	-3.47382400
C	-3.51080100	1.76437600	-2.22782100
C	-4.07860300	-0.43656100	-1.35007300

C	-4.66743700	-0.73569600	-2.59256000
C	-0.83582600	3.35039900	-0.96031500
C	-2.04699700	3.87998900	-1.40718800
C	-2.34947900	5.22917000	-1.17361900
C	-1.40227400	6.07936700	-0.61389600
C	-0.15322300	5.56237600	-0.27646000
C	0.15397100	4.19599600	-0.41500200
H	-5.14976800	-1.70097400	-2.71274300
H	0.60786300	6.22098600	0.13124400
C	-3.15030300	3.24664700	-2.24425500
C	-2.86960100	3.44893700	-3.77183700
H	-1.84679900	3.11827900	-3.98614000
H	-2.95277900	4.49655100	-4.07765800
H	-3.78126900	6.12755700	-2.53481900
H	-4.31246600	6.12674900	-0.85683400
C	-3.45837000	0.82123800	-1.19773100
H	-5.05037900	-0.12634200	-4.62449800
H	-1.62265900	7.13091400	-0.44736700
C	-3.87597500	2.51866500	-4.47888300
H	-3.51274700	2.15860800	-5.44843300
H	-4.82962300	3.03073900	-4.67080500
C	-3.76607600	5.54104100	-1.60530000
C	-4.36724000	4.13423900	-1.81674700
H	-4.76261900	3.75396000	-0.86776900
H	-5.17991800	4.11316300	-2.54970500
C	1.51560500	3.73669200	-0.00050800
C	1.94765300	3.95527700	1.33418300
C	2.42230500	3.20922100	-0.95555200
C	1.07277200	4.43112100	2.36575600
C	3.32257100	3.69388700	1.69764500
C	3.77655000	2.89036000	-0.55915100
C	1.53696000	4.70911300	3.62667200
H	0.02146500	4.55685100	2.13827200
C	3.76752400	3.99896800	3.02337900
C	4.19437400	3.15530100	0.74775600
C	2.90837500	4.51039700	3.95903700
H	0.85025200	5.07891700	4.38380200
H	4.81152200	3.81711900	3.26810200
H	5.22426200	2.94563800	1.02921900
H	3.26276300	4.75116700	4.95808700
C	-4.20682800	-1.46259000	-0.26907500
C	-3.69500300	-2.76713700	-0.48970800
C	-4.98494200	-1.19703400	0.88684000
C	-2.82555400	-3.08384500	-1.58588700

C	-4.04545700	-3.83915900	0.41458200
C	-5.26263900	-2.26412500	1.82299200
C	-2.40707000	-4.36949100	-1.81988600
H	-2.47739700	-2.28072100	-2.22429000
C	-3.61053600	-5.17089100	0.12069800
C	-4.80725700	-3.55709700	1.55112200
C	-2.82975300	-5.43522100	-0.97306600
H	-1.73277300	-4.57386500	-2.64533600
H	-3.91648400	-5.97022600	0.79206200
H	-5.06121200	-4.36449500	2.23537200
H	-2.51454400	-6.45269300	-1.19087300
C	2.96589000	2.46756500	-3.22152500
H	2.66652800	2.31178700	-4.25444200
C	2.07263100	2.99863700	-2.32832600
H	1.07732500	3.26491800	-2.66166200
C	4.28402000	2.11509000	-2.81482400
H	4.97007800	1.66795000	-3.52763300
C	4.67637200	2.33276500	-1.52182000
H	5.68546100	2.08507300	-1.19982900
C	-6.29767100	0.31159200	2.29414700
H	-6.71091000	1.29939300	2.47963200
C	-6.53857200	-0.73513900	3.22856400
H	-7.12802600	-0.53737500	4.11996800
C	-6.03855300	-1.98657000	2.99222400
H	-6.22838800	-2.80129600	3.68743100
C	-5.55464100	0.08705200	1.16499800
H	-5.38957800	0.89640300	0.46498500
C	0.92072300	0.35722300	4.79542000
C	0.43687400	-1.12495500	4.68474000
H	0.07506200	-1.42582500	5.68288000
H	-0.45308600	-1.15277800	4.05202600
C	0.82012600	-3.30013800	3.40551100
C	-0.08240800	-3.01525800	2.35706500
C	1.24386600	-4.63633000	3.58594100
C	-0.51270200	-4.02482600	1.50398500
H	-0.39671800	-1.99698300	2.15432700
C	0.77501400	-5.64806400	2.75659200
H	1.90518700	-4.88351600	4.41064400
C	-0.09520600	-5.34220200	1.70657000
H	-1.16792100	-3.77880100	0.67734700
H	1.09034200	-6.67368400	2.92584400
H	-0.45242400	-6.12540400	1.04472300
C	1.35825600	-2.23356000	4.25150400
C	1.90904200	0.75213300	3.65992400

H	2. 92772900	0. 45397600	3. 90447700
H	1. 90570000	1. 84358200	3. 57664200
N	1. 57761500	0. 20333800	2. 34609200
C	2. 41363200	-0. 45217900	1. 52122800
N	1. 93961300	-0. 69719800	0. 28039800
C	2. 53667000	-1. 36336500	-0. 81189900
C	3. 89179400	-1. 25499700	-1. 14678700
C	1. 67350000	-2. 08684100	-1. 64584600
C	4. 37448900	-1. 90630500	-2. 28027500
C	2. 17446900	-2. 72839600	-2. 77791100
H	0. 61409700	-2. 11622300	-1. 41431800
C	3. 52842700	-2. 65537700	-3. 09990000
H	3. 91483100	-3. 15685700	-3. 97907900
C	1. 23420800	-3. 54541400	-3. 62395600
C	5. 81283100	-1. 72932600	-2. 68811000
F	0. 96591600	-4. 74812000	-3. 05580300
F	1. 73809200	-3. 79438400	-4. 85117000
F	0. 04232200	-2. 92755100	-3. 79107300
F	5. 94162800	-0. 80012100	-3. 66975000
F	6. 33781700	-2. 87561300	-3. 17556500
F	6. 59166600	-1. 32670100	-1. 66272600
S	3. 97323400	-1. 02723100	2. 05281500
H	4. 55861600	-0. 65043800	-0. 54968900
H	0. 92754000	-0. 49642000	0. 10563800
H	0. 70356100	0. 60230600	1. 93868000
C	2. 72482600	-2. 25629900	4. 57098600
H	3. 08039600	-1. 63849400	5. 39179900
H	3. 24623500	-1. 67922200	3. 52499300
H	3. 24752700	-3. 20757200	4. 46698300
C	-0. 35131100	1. 23262300	4. 72028400
H	-1. 07509300	0. 92462100	5. 48516900
H	-0. 09752700	2. 28283300	4. 90190700
H	-0. 83185000	1. 17623800	3. 73891900
C	1. 61532100	0. 65568500	6. 14126100
H	1. 92320400	1. 70702700	6. 17857600
H	0. 92738700	0. 48374600	6. 97718200
H	2. 51108700	0. 05034400	6. 31329400
O	-0. 77579700	1. 46482400	1. 46486200

TS-EF-1R'

l imaginary frequencies

H = -4333. 068995

G = -4333. 244472

E(M06-2X-DCM) = -4333. 860937

O	-2.73607500	-0.94156900	0.27477500
O	-2.29654300	1.12692600	-1.21337100
P	-1.50996100	0.06375300	-0.22312900
O	-0.52808700	-0.67284000	-1.09431000
C	-4.43158900	-3.31723400	-2.73002200
C	-4.87346800	-2.01556200	-2.51821300
C	-4.37029600	-1.25577300	-1.45215400
C	-2.88549500	-3.08785100	-0.84607000
C	-3.47092700	-3.85077300	-1.87112000
C	-3.35771200	1.87508300	-0.72709300
C	-4.64101800	1.32209300	-0.70651300
C	-5.69236900	2.03886600	-0.11381700
C	-5.49816400	3.33205300	0.35845100
C	-4.23550400	3.90791100	0.23859300
C	-3.14243500	3.19778100	-0.28802600
H	-3.13590800	-4.87508100	-2.00675400
H	-4.07278500	4.92782600	0.57469700
C	-5.17959000	0.02638100	-1.30688200
C	-5.65144400	0.22397300	-2.78640200
H	-4.84444600	0.70490400	-3.35097000
H	-6.53888900	0.86044100	-2.86251700
H	-7.67458300	1.54239600	-0.83929000
H	-7.47054000	1.26646500	0.88753900
C	-3.32949500	-1.76067500	-0.67409200
H	-4.82678400	-3.91550000	-3.54725700
H	-6.31531000	3.89068500	0.80815300
C	-5.87630600	-1.21005900	-3.31668400
H	-5.71231800	-1.29105300	-4.39745400
H	-6.90459800	-1.55006600	-3.12873600
C	-6.95546400	1.20726700	-0.07833500
C	-6.42711800	-0.20797400	-0.38865400
H	-6.09379300	-0.68902400	0.53821200
H	-7.17221700	-0.86069700	-0.85411800
C	-1.82907000	3.90767400	-0.38527800
C	-1.18811200	4.35520400	0.79686300
C	-1.29919900	4.25645600	-1.65278400
C	-1.63796000	3.98621000	2.10658500
C	-0.03036000	5.21553500	0.70516700
C	-0.11449500	5.08229700	-1.73022000
C	-1.02548800	4.46998600	3.23417600
H	-2.46981500	3.29820700	2.19433700
C	0.57468900	5.70368900	1.90623400
C	0.47596500	5.55282700	-0.55329800
C	0.08910400	5.35211300	3.13653900

H	-1.39232300	4.17725600	4.21478800
H	1.43572900	6.36209400	1.81702300
H	1.34639100	6.20320500	-0.61918000
H	0.55554300	5.73480400	4.04068500
C	-1.84001400	-3.71528800	0.01982400
C	-0.62036900	-4.15524000	-0.55327200
C	-2.10152000	-3.95129500	1.39365800
C	-0.27682900	-3.91536800	-1.92437100
C	0.34184200	-4.86249100	0.26217500
C	-1.11900800	-4.63795000	2.20244500
C	0.90085500	-4.37388900	-2.45582900
H	-0.95638200	-3.33567600	-2.53662600
C	1.55896600	-5.32452900	-0.33181200
C	0.07006400	-5.07990900	1.61529100
C	1.83015900	-5.09652600	-1.65318400
H	1.14696600	-4.16302300	-3.49255300
H	2.26708400	-5.85825300	0.29748400
H	0.80060400	-5.60743300	2.22516600
H	2.75908100	-5.44897900	-2.09308800
C	-1.36861000	4.20746200	-4.09567000
H	-1.84731000	3.88058100	-5.01472100
C	-1.90530200	3.85338100	-2.88588100
H	-2.80687600	3.25382400	-2.85423100
C	-0.18865100	5.00123800	-4.16493900
H	0.22363300	5.27011600	-5.13376400
C	0.41448500	5.42836100	-3.01349800
H	1.30895200	6.04611700	-3.05130000
C	-3.54648500	-3.79758000	3.36238300
H	-4.48465100	-3.48893200	3.81590700
C	-2.56539500	-4.45508800	4.15875700
H	-2.76109800	-4.64071400	5.21174300
C	-1.38994100	-4.86640800	3.58915200
H	-0.63818500	-5.38540500	4.17982300
C	-3.32315700	-3.55984000	2.03090400
H	-4.08609200	-3.06853300	1.43881500
C	0.19674400	-0.24338200	4.53107500
C	1.09566300	1.02527900	4.30292700
H	1.12758900	1.57356600	5.25868600
H	0.57936200	1.69505500	3.61333900
C	3.06359700	1.76516400	2.81568400
C	2.25053700	2.20558400	1.74602000
C	4.43466700	2.11889300	2.79958600
C	2.80385300	2.91838500	0.68548600
H	1.20003100	1.93811000	1.69451100

C	4. 97462200	2. 85025500	1. 74942100
H	5. 07238100	1. 84761800	3. 63451500
C	4. 16255200	3. 23863100	0. 67962700
H	2. 16709400	3. 21799600	-0. 14008800
H	6. 02859100	3. 11121900	1. 75839400
H	4. 59043400	3. 78649800	-0. 15479700
C	2. 53458400	0. 89082500	3. 86873400
C	0. 53316600	-1. 40101800	3. 54638400
H	1. 34918700	-2. 01602100	3. 92424200
H	-0. 34626700	-2. 05147100	3. 46730600
N	0. 89330100	-0. 94669100	2. 20696500
C	1. 94108100	-1. 35077400	1. 47232800
N	1. 87765200	-1. 05806800	0. 15543300
C	2. 91401700	-0. 97489500	-0. 79836800
C	4. 20796400	-0. 53557700	-0. 49678800
C	2. 56994500	-1. 24398600	-2. 12953900
C	5. 15004500	-0. 40720100	-1. 51672500
C	3. 52829700	-1. 12213200	-3. 13406600
H	1. 55279000	-1. 53591700	-2. 36409700
C	4. 82729200	-0. 70775200	-2. 84010400
H	5. 56692100	-0. 61021500	-3. 62467800
C	3. 15250600	-1. 50362100	-4. 54176500
C	6. 50407600	0. 15380800	-1. 17533300
F	4. 01443800	-1. 00088600	-5. 45205400
F	3. 15147200	-2. 85224800	-4. 70513800
F	1. 91655400	-1. 07431000	-4. 86639900
F	6. 96777800	-0. 32515600	0. 00026600
F	7. 42613300	-0. 12351000	-2. 12076600
F	6. 46409500	1. 50644100	-1. 04925100
S	3. 28998600	-2. 19586100	2. 18205300
H	4. 47852600	-0. 28482400	0. 51949700
H	0. 92504300	-0. 88942500	-0. 25212900
H	0. 17936200	-0. 35096500	1. 73256300
C	3. 36984200	-0. 10022700	4. 40613500
H	3. 06395400	-0. 59093600	5. 32645200
H	3. 28895900	-1. 05668200	3. 49874400
H	4. 44747000	0. 03120600	4. 31309500
C	-1. 26621100	0. 21205600	4. 32504500
H	-1. 50625300	1. 04467200	4. 99817400
H	-1. 95440600	-0. 61052300	4. 55215500
H	-1. 44953700	0. 53475200	3. 29561400
C	0. 31579100	-0. 80436300	5. 96404100
H	-0. 33867200	-1. 67616200	6. 08134000
H	0. 00132200	-0. 05532400	6. 69986600

H	1.33082900	-1.12402400	6.22136500
O	-1.01922800	0.72824600	1.04342900

TS-1-1S

l imaginary frequencies

H = -4333.071361

G = -4333.246591

E(M06-2X-DCM) = -4333.864626

C	-1.24939300	-2.70181500	3.90488900
C	-0.55669400	-1.55088200	4.73252000
H	-1.30681600	-1.20086200	5.44970900
H	0.24061200	-2.02257400	5.31184300
C	1.38423000	-0.24702900	3.63752600
C	2.37734600	-1.05993000	4.23148700
C	1.79256300	0.68241600	2.65011300
C	3.71311900	-0.93683400	3.86783000
H	2.11767700	-1.77952200	4.99800400
C	3.12283500	0.77868400	2.26716500
H	1.05649600	1.30160100	2.15085000
C	4.08940200	-0.02402800	2.88160500
H	4.45714800	-1.56967900	4.34095800
H	3.40672000	1.47656700	1.48742600
H	5.13099700	0.05556700	2.58361600
C	-0.02172400	-0.33221400	4.02084400
C	-0.25243800	-3.47776100	3.01353200
H	-0.77434000	-4.35793800	2.60954500
H	0.57975100	-3.85542800	3.61320700
N	0.30722400	-2.69583600	1.92830200
C	1.50160100	-2.96023900	1.32356700
N	1.70243700	-2.11868500	0.25327200
C	2.76244500	-1.91012900	-0.63117700
C	3.93450700	-2.67749500	-0.72011700
C	2.59858500	-0.81924700	-1.50961900
C	4.90545500	-2.34315800	-1.66688500
C	3.57683300	-0.50981000	-2.44726300
H	1.70139800	-0.21095000	-1.44297600
C	4.74640300	-1.26758500	-2.53875700
H	5.51011900	-1.02576900	-3.26721500
C	3.33701700	0.62216400	-3.40863000
C	6.18915300	-3.13219100	-1.69527500
F	2.61555600	0.22851600	-4.48740500
F	4.48911800	1.14683700	-3.87786500
F	2.64043200	1.63816900	-2.83497900
F	6.77857400	-3.09226700	-2.91237300

F	5.99535000	-4.42956600	-1.38126400
F	7.09057100	-2.64330000	-0.80922300
S	2.56048100	-4.15976000	1.86508300
C	-1.77053800	-3.71255500	4.95059200
H	-2.49470600	-3.24176500	5.62491500
H	-2.27271400	-4.54974600	4.45387700
H	-0.95540400	-4.12288900	5.55874400
C	-2.44970500	-2.16990300	3.10302500
H	-2.95579300	-2.99427800	2.59035600
H	-3.17981600	-1.69518300	3.76955900
H	-2.17536700	-1.43229900	2.34551700
H	4.07435800	-3.52014800	-0.05767300
C	-0.90097000	0.74871900	3.78163600
H	0.93148200	-1.46172500	0.09837100
H	-1.84119200	0.71538900	4.33202300
H	-0.44853700	1.74120200	3.77242000
H	-0.32711200	-2.08006100	1.41931800
H	-1.34814200	0.79892000	2.57138700
O	-0.45691300	1.75144400	-0.61550500
O	-2.74650300	0.54370600	-0.87721500
P	-1.43829100	0.63842000	0.10552400
O	-0.65236400	-0.63828300	0.13315500
C	-2.06517800	5.49252600	-1.63925600
C	-2.23803000	4.39282600	-2.47198800
C	-1.65000700	3.15676300	-2.16316000
C	-0.71068600	4.12026600	-0.13255200
C	-1.28126400	5.35253000	-0.49686500
C	-2.54057400	-0.06910900	-2.12029500
C	-1.99343400	0.68080000	-3.15926000
C	-1.58010200	0.03740500	-4.33498300
C	-1.84150200	-1.31542300	-4.52546700
C	-2.51921100	-2.01878700	-3.53029400
C	-2.86392600	-1.42790100	-2.30099800
H	-1.10207900	6.21025400	0.14484900
H	-2.76786200	-3.06452400	-3.68427900
C	-1.84372500	2.18669100	-3.32223900
C	-3.13679700	2.78401200	-3.97749200
H	-3.23942800	2.49734900	-5.02855500
H	-4.01215700	2.40093200	-3.44024600
H	0.09269800	0.60390900	-5.60805400
H	-1.46264500	1.24551400	-6.13596800
C	-0.94976700	3.00945600	-0.96426500
H	-2.51962200	6.45064500	-1.87823200
H	-1.53586300	-1.81989700	-5.43854700

C	-3.02293700	4.30605500	-3.76141400
H	-2.47993400	4.78886100	-4.58616700
H	-3.99901500	4.80021100	-3.69551900
C	-0.86040800	1.00717200	-5.24833200
C	-0.65946600	2.24460500	-4.34265200
H	-0.63460700	3.18787400	-4.89772600
H	0.28686600	2.15058800	-3.80020700
C	-3.58615000	-2.25290700	-1.28379400
C	-4.92273300	-1.93279600	-0.93137600
C	-2.97748900	-3.42396200	-0.76516400
C	-5.61351900	-0.78924300	-1.44696700
C	-5.65525300	-2.80420800	-0.04007200
C	-3.73758900	-4.30701600	0.09191600
C	-6.90499300	-0.50858600	-1.08507800
H	-5.10072900	-0.13706800	-2.14370900
C	-6.99982600	-2.47273200	0.31733600
C	-5.04933800	-3.97003600	0.43597300
C	-7.60988300	-1.35520500	-0.18356200
H	-7.40049500	0.36849900	-1.49269700
H	-7.52946000	-3.13803400	0.99538800
H	-5.61636400	-4.63593500	1.08385900
H	-8.63251100	-1.11485800	0.09448800
C	0.17806600	4.11232800	1.07327400
C	1.58551000	4.08633400	0.90086700
C	-0.37512800	4.31429000	2.36066400
C	2.20761900	3.85802600	-0.36896300
C	2.44896200	4.31764700	2.03777600
C	0.50050500	4.52869400	3.49216900
C	3.57163400	3.85698600	-0.50786600
H	1.58304300	3.67370400	-1.23452700
C	3.86672300	4.32941100	1.84632300
C	1.88482800	4.53520800	3.29825800
C	4.41623700	4.10617300	0.61195700
H	4.01038700	3.65787800	-1.48114300
H	4.50010000	4.51645900	2.71034500
H	2.53938000	4.71692500	4.14837300
H	5.49496600	4.11564700	0.48103000
C	-1.06747800	-4.93928400	-0.55414900
H	-0.03018400	-5.17891300	-0.76933600
C	-1.61746700	-3.78227100	-1.04273000
H	-1.01210200	-3.10789500	-1.63609000
C	-1.83596700	-5.82558600	0.25453100
H	-1.38546200	-6.74337100	0.62243200
C	-3.12986100	-5.51022600	0.57280400

H	-3.72521600	-6.17143200	1.19871100
C	-2.29577000	4.51794100	3.85722600
H	-3.37095100	4.50189900	4.01344800
C	-1.42962600	4.74494100	4.96573000
H	-1.85187800	4.91277600	5.95293100
C	-0.07261100	4.74440700	4.78590400
H	0.59919500	4.91118100	5.62474500
C	-1.78816000	4.31014600	2.60117900
H	-2.45607200	4.11127500	1.77186600
O	-1.98193900	1.19336800	1.42456000

TS-1-1R

l imaginary frequencies

H = -4333.068995

G = -4333.244472

E(M06-2X-DCM) = -4333.860704

O	-0.56600000	1.82170400	-1.16597200
O	-2.81783900	0.98268300	-0.18352400
P	-1.19561000	0.78894200	-0.07437000
O	-0.87827900	1.29268100	1.35944000
C	0.76960200	0.95905600	4.91273100
C	-0.06726400	-0.35842400	5.08905300
H	-0.89204600	-0.11578100	5.77164100
H	0.58310800	-1.06118300	5.60964400
C	-0.16609400	-2.31828100	3.41938400
C	0.54528100	-3.18106300	4.28422800
C	-0.41148200	-2.76317300	2.09918600
C	0.97713000	-4.43119900	3.85416700
H	0.73442500	-2.90219800	5.31360400
C	0.05021100	-3.99951000	1.66573400
H	-0.91324800	-2.11732000	1.38755300
C	0.73976400	-4.84163800	2.54229400
H	1.51034400	-5.07946100	4.54317900
H	-0.13019600	-4.30335700	0.64043900
H	1.09566400	-5.80986400	2.20128400
C	-0.66876100	-1.01555000	3.86852100
C	1.99013000	0.74065900	3.98799700
H	2.54479500	1.68736500	3.91952600
H	2.66647000	0.01057000	4.43690300
N	1.68790500	0.24832300	2.64813900
C	2.54260400	-0.56390600	1.94547800
N	2.09464000	-0.81675600	0.66876100
C	2.72786800	-1.48848300	-0.39452200
C	4.11492500	-1.50602900	-0.59366700

C	1. 89519400	-2. 09682100	-1. 34761200
C	4. 64444000	-2. 13108000	-1. 72244800
C	2. 44552700	-2. 72429600	-2. 46330600
H	0. 81931700	-2. 04301700	-1. 22594900
C	3. 82539800	-2. 75364100	-2. 66370000
H	4. 25035400	-3. 23842200	-3. 53370400
C	1. 53174200	-3. 42994500	-3. 42727000
C	6. 12485900	-2. 03357000	-1. 97107200
F	0. 35263600	-2. 78413800	-3. 58127500
F	2. 08397600	-3. 56070600	-4. 65302800
F	1. 22566300	-4. 68533400	-3. 00276400
F	6. 57015100	-3. 00730500	-2. 79500300
F	6. 45199900	-0. 84894000	-2. 56017200
F	6. 84160500	-2. 10345500	-0. 83118100
S	3. 94502500	-1. 21922100	2. 61404600
H	4. 77048800	-1. 03255800	0. 12211100
C	-1. 74044800	-0. 38226900	3. 21586600
H	1. 11101700	-0. 61928300	0. 46904900
H	-2. 26746000	0. 37921100	3. 79017700
H	-2. 39820600	-1. 00107900	2. 60692400
H	1. 02139400	0. 79353500	2. 10243200
H	-1. 23908400	0. 42135700	2. 27312400
C	-4. 53134600	-0. 16063800	-3. 83551500
C	-3. 98029400	1. 10556100	-3. 67546400
C	-3. 47879600	1. 51789300	-2. 43073200
C	-4. 01877200	-0. 67208600	-1. 49743800
C	-4. 57308100	-1. 02203300	-2. 74118400
C	-0. 81454600	3. 19353500	-1. 16405200
C	-2. 02817900	3. 67257700	-1. 65711500
C	-2. 33021100	5. 03701800	-1. 52149700
C	-1. 37623800	5. 93056400	-1. 04755200
C	-0. 11490500	5. 45006900	-0. 69995800
C	0. 19291500	4. 07767900	-0. 72184100
H	-5. 02285600	-2. 00483500	-2. 84453000
H	0. 65615400	6. 14489100	-0. 38192600
C	-3. 12048800	2. 99903300	-2. 48490200
C	-2. 81029100	3. 14946100	-4. 01475000
H	-1. 78288900	2. 81482900	-4. 19872300
H	-2. 88943200	4. 18555100	-4. 35727000
H	-3. 76649900	5. 86139700	-2. 92443500
H	-4. 29751100	5. 93598300	-1. 24876200
C	-3. 44168400	0. 60672200	-1. 37683200
H	-4. 92685200	-0. 47863100	-4. 79676700
H	-1. 59767400	6. 99191200	-0. 96758300

C	-3.80026000	2.19296100	-4.71075800
H	-3.41828000	1.80657200	-5.66244300
H	-4.75294500	2.69386100	-4.93351600
C	-3.74843700	5.31863700	-1.96918500
C	-4.34395900	3.90099300	-2.11338600
H	-4.74869400	3.56685500	-1.15105400
H	-5.14814600	3.84024400	-2.85311300
C	1.56268000	3.62630600	-0.32545700
C	2.07553800	3.95915500	0.95682900
C	2.38894500	2.95122000	-1.26290900
C	1.31512800	4.65820800	1.95136600
C	3.43306200	3.59572600	1.30093500
C	3.72322100	2.54595300	-0.88049400
C	1.87057500	5.03386400	3.14804600
H	0.27787700	4.89526500	1.74781100
C	3.96762800	3.98659800	2.56930200
C	4.20820500	2.87932700	0.38626000
C	3.21915000	4.70336800	3.46402000
H	1.27083300	5.58255800	3.86988700
H	4.99319000	3.70842500	2.79960000
H	5.21914800	2.58702800	0.66154000
H	3.64377100	5.01225100	4.41549000
C	-4.11177200	-1.66138700	-0.37928300
C	-3.48556000	-2.92670700	-0.51224000
C	-4.93656400	-1.39114800	0.74236600
C	-2.58072900	-3.23811400	-1.58004400
C	-3.74571200	-3.95949800	0.46572200
C	-5.13695000	-2.41503300	1.74443100
C	-2.03778800	-4.49052700	-1.71309300
H	-2.30275000	-2.45724100	-2.27728000
C	-3.17409500	-5.25775500	0.28067700
C	-4.55216200	-3.67281200	1.57022500
C	-2.35744100	-5.52372700	-0.78505400
H	-1.33899900	-4.69056900	-2.51877500
H	-3.40285600	-6.02885500	1.01262800
H	-4.73670500	-4.45036900	2.30888900
H	-1.93218800	-6.51517000	-0.91729200
C	2.79762700	1.99816700	-3.47811000
H	2.45608000	1.80016700	-4.49060400
C	1.98149500	2.67152700	-2.60702100
H	1.00843100	3.00901200	-2.94273400
C	4.08664600	1.55047800	-3.07443100
H	4.71027100	0.98879700	-3.76322000
C	4.53604500	1.82793300	-1.81268500

H	5.52221500	1.49997700	-1.49596700
C	-6.40588600	0.08396100	2.02581800
H	-6.91068700	1.03986100	2.13742000
C	-6.57468100	-0.91785300	3.02362700
H	-7.20007600	-0.71678800	3.88927100
C	-5.96037700	-2.13211900	2.87974800
H	-6.09277900	-2.91326200	3.62483500
C	-5.62103600	-0.14614300	0.92621100
H	-5.51537000	0.62602200	0.17345800
C	1.34027700	1.29033200	6.31089700
H	0.53323000	1.48676500	7.02625900
H	1.95339100	0.47117600	6.70445700
H	1.96837700	2.18686800	6.26419200
C	-0.09662900	2.15424700	4.47312500
H	-0.95431500	2.27540100	5.14704900
H	0.49712100	3.07198500	4.52274800
H	-0.47382900	2.07896500	3.45291800
O	-0.71895500	-0.58307000	-0.41782700

INT-10

0 imaginary frequencies

H = -4333.075321

G = -4333.249265

E(M06-2X-DCM) = -4333.871089

C	-0.96701500	-4.41294700	1.99471600
C	0.34126700	-4.19703900	2.85131200
H	0.04815800	-4.32809100	3.90287300
H	1.01583300	-5.01474500	2.59586100
C	2.37505700	-2.71717200	2.30121600
C	3.21222000	-3.82652100	1.99298100
C	2.92484400	-1.41108100	2.13502100
C	4.53377300	-3.63739200	1.60286500
H	2.84619900	-4.83835500	2.10202000
C	4.22244400	-1.23396200	1.69190500
H	2.31299600	-0.53798300	2.32641700
C	5.03714100	-2.34832400	1.43631400
H	5.15719800	-4.50018400	1.39140000
H	4.60469200	-0.22982600	1.54065800
H	6.05312000	-2.20288500	1.08111600
C	1.02646100	-2.86959100	2.76803700
C	-0.58808700	-4.33338000	0.50086100
H	-1.49831700	-4.45395500	-0.10060200
H	0.09525100	-5.14291500	0.23731200
N	0.05826500	-3.08177100	0.14617200

C	1. 15559800	-2. 99436200	-0. 68195300
N	1. 35037000	-1. 70950800	-1. 10131300
C	2. 40028100	-1. 07313000	-1. 77203200
C	3. 67779200	-1. 60811000	-1. 98433400
C	2. 13372700	0. 24411800	-2. 19562400
C	4. 66094700	-0. 82535200	-2. 59431800
C	3. 12212600	0. 99717100	-2. 81741400
H	1. 15573500	0. 67712800	-2. 00902300
C	4. 40192300	0. 47366600	-3. 02246000
H	5. 17496900	1. 06703000	-3. 49437500
C	2. 79346800	2. 37766000	-3. 32017100
C	6. 05110100	-1. 39326400	-2. 69702200
F	2. 33670800	2. 35665600	-4. 59184000
F	3. 87982600	3. 18846600	-3. 30957000
F	1. 83976700	2. 97995000	-2. 57080400
F	6. 82108600	-0. 71496700	-3. 57307400
F	6. 04492700	-2. 68841800	-3. 07451600
F	6. 69004800	-1. 34575400	-1. 49503700
S	2. 11666700	-4. 33232800	-1. 06531200
C	-1. 45440200	-5. 84760600	2. 28137800
H	-1. 76658800	-5. 95651200	3. 32623500
H	-2. 31835300	-6. 08569100	1. 65119600
H	-0. 67493700	-6. 59134500	2. 07734200
C	-2. 10638300	-3. 43395100	2. 33572700
H	-2. 99845100	-3. 70662300	1. 76060200
H	-2. 37147900	-3. 49430400	3. 39824500
H	-1. 88476100	-2. 38874600	2. 10698200
H	3. 89641900	-2. 62075900	-1. 67757200
C	0. 33347200	-1. 71814000	3. 40750300
H	0. 55426000	-1. 07947500	-0. 89119300
H	-0. 47205400	-2. 05753800	4. 05960000
H	1. 02535800	-1. 10545800	3. 99223800
H	-0. 54919400	-2. 24773800	0. 12443400
H	-0. 14779100	-1. 02671200	2. 68422700
O	-0. 51000700	1. 83954400	0. 12725600
O	-2. 98042100	1. 03651400	0. 07343900
P	-1. 46785600	0. 52996500	0. 51745600
O	-1. 00122200	-0. 54435800	-0. 44657100
C	-1. 53578500	5. 53093300	1. 83839600
C	-2. 13804800	5. 09809000	0. 66248000
C	-1. 75214700	3. 89305000	0. 05646000
C	-0. 15377200	3. 51181300	1. 85379000
C	-0. 53470900	4. 74707100	2. 40646700
C	-3. 21952600	1. 20437400	-1. 28394900

C	-2.85619100	2.40282100	-1.89654200
C	-2.92378200	2.51896200	-3.29259100
C	-3.46726400	1.49470600	-4.06112900
C	-3.94010900	0.34912800	-3.42065600
C	-3.81162800	0.16713100	-2.03266500
H	-0.03462400	5.08136300	3.31100800
H	-4.39829100	-0.44414200	-4.00432400
C	-2.45581300	3.74119100	-1.28900300
C	-3.72830400	4.62250800	-1.04002700
H	-4.18271100	4.97221100	-1.97224500
H	-4.47411600	4.01765500	-0.51138500
H	-1.64997600	3.72402700	-4.59109400
H	-3.12070400	4.53718900	-4.06731600
C	-0.80608300	3.07574100	0.68255500
H	-1.83409900	6.46498600	2.30787400
H	-3.53295600	1.58235700	-5.14280300
C	-3.24545500	5.76359500	-0.12314300
H	-2.86200200	6.61225500	-0.70744300
H	-4.04069300	6.15811000	0.51987400
C	-2.33545200	3.83951100	-3.74357200
C	-1.62172400	4.34367500	-2.46790200
H	-1.54918100	5.43485400	-2.41401900
H	-0.60502600	3.93752700	-2.43010300
C	-4.33207800	-1.09229800	-1.41557600
C	-5.44642800	-1.04556200	-0.53923900
C	-3.78136900	-2.34329200	-1.79121200
C	-6.07418100	0.17966200	-0.14546900
C	-6.01209600	-2.27572800	-0.03246700
C	-4.38567200	-3.56699500	-1.31243600
C	-7.14967000	0.19269900	0.70331100
H	-5.68655100	1.11379600	-0.53367100
C	-7.13214900	-2.21861600	0.85508300
C	-5.47554900	-3.50046500	-0.44016500
C	-7.68525700	-1.02126800	1.21912700
H	-7.60223600	1.13933600	0.98608100
H	-7.53867200	-3.15520900	1.23008100
H	-5.92721300	-4.42371100	-0.08149700
H	-8.53700500	-0.99128100	1.89342900
C	0.96741000	2.78593600	2.53526000
C	2.27136700	2.83413500	1.98162000
C	0.76381300	2.21870900	3.81693300
C	2.54270100	3.37808700	0.68478000
C	3.39477400	2.34766700	2.75241700
C	1.89501100	1.73329300	4.57647600

C	3.81781600	3.43603900	0.18497300
H	1.71594600	3.74091000	0.08616000
C	4.71229100	2.44047300	2.20022300
C	3.17855400	1.81857600	4.02852700
C	4.92110400	2.96630000	0.95308400
H	3.99016700	3.83581700	-0.80915200
H	5.54801700	2.09073200	2.80295900
H	4.03014000	1.47353600	4.61223600
H	5.92678600	3.03285000	0.54652100
C	-2.14549200	-3.68406200	-3.02152600
H	-1.26616000	-3.74299100	-3.65689100
C	-2.62746800	-2.46035900	-2.63396900
H	-2.12155700	-1.55541600	-2.94650200
C	-2.77761700	-4.88558500	-2.58831100
H	-2.38965600	-5.84614700	-2.91686500
C	-3.85795100	-4.82431700	-1.74862000
H	-4.34272900	-5.73380000	-1.39984900
C	-0.70323200	1.56780600	5.65840500
H	-1.70165700	1.47979500	6.07775900
C	0.41667200	1.11324500	6.41260000
H	0.26464900	0.70250700	7.40753300
C	1.67695300	1.18868600	5.88237500
H	2.54005500	0.84255600	6.44694600
C	-0.53649700	2.10001300	4.40665700
H	-1.39797600	2.40751500	3.82794500
O	-1.49399100	0.28199900	1.99180500

TS-1-1S'

l imaginary frequencies

H = -4333.074824

G = -4333.249823

E(M06-2X-DCM) = -4333.870171

C	0.66383100	4.41783000	2.18800800
C	-0.60615800	4.07776300	3.03909700
H	-0.32116200	4.07673600	4.10069500
H	-1.31416300	4.89471700	2.89398300
C	-2.65409900	2.60291000	2.46179400
C	-3.53561100	3.70857100	2.38125200
C	-3.19852000	1.31035600	2.24499700
C	-4.89647700	3.52416800	2.15856100
H	-3.16935200	4.71715600	2.52206900
C	-4.54919300	1.13556300	1.98301000
H	-2.55587000	0.43846200	2.27309900
C	-5.40619600	2.24198400	1.95464400

H	-5.55489600	4.38663200	2.12283000
H	-4.93135700	0.13543200	1.80465300
H	-6.46677400	2.10285100	1.76415400
C	-1.23678700	2.74400500	2.75406600
C	0.22157900	4.25273000	0.72437500
H	1.08290500	4.32712900	0.05056600
H	-0.49570800	5.02717900	0.44728100
N	-0.43112700	2.95588500	0.53590200
C	-1.47605400	2.80001900	-0.39860700
N	-1.54919600	1.50935000	-0.81579800
C	-2.44999900	0.82945800	-1.65055700
C	-3.68146800	1.32417700	-2.09981500
C	-2.05670400	-0.47322800	-2.01681700
C	-4.49295800	0.52011300	-2.90460500
C	-2.87926900	-1.25143500	-2.82144200
H	-1.11455800	-0.87256500	-1.65357200
C	-4.10773300	-0.76418700	-3.27644400
H	-4.74815200	-1.37461700	-3.90152200
C	-2.42996100	-2.62142400	-3.25482900
C	-5.84658100	1.04183600	-3.31246300
F	-1.87033400	-2.60455400	-4.48459900
F	-3.46844600	-3.49064200	-3.31097500
F	-1.51360700	-3.14998000	-2.41105900
F	-6.31215300	0.42725800	-4.42172700
F	-5.82298300	2.36809700	-3.56015800
F	-6.76648800	0.84248400	-2.33676400
S	-2.48208500	4.07308300	-0.82407600
C	1.03677900	5.89007000	2.44005200
H	1.35553000	6.04208000	3.47763700
H	1.86855900	6.18817400	1.79215300
H	0.19506600	6.56330900	2.23869800
C	1.89258500	3.54073600	2.50489200
H	2.75049300	3.89935500	1.92507600
H	2.15984800	3.61190700	3.56621600
H	1.76669600	2.48218200	2.26403100
H	-3.99404800	2.32369900	-1.83582900
C	-0.50181000	1.54576300	3.28924500
H	-0.70904400	0.94539400	-0.57583600
H	0.36237100	1.84716600	3.87975700
H	-1.16127200	0.95228100	3.92973800
H	0.24184800	2.16774500	0.48479000
H	-0.10640600	0.86128800	2.52930300
O	0.67061800	-1.83087200	0.19092500
O	3.05422200	-0.81932700	0.00740400

P	1. 55787100	-0. 48359800	0. 62842700
O	0. 90809900	0. 62141700	-0. 19144200
C	2. 04451400	-5. 45844800	1. 78061400
C	2. 57184100	-4. 95505600	0. 59649100
C	2. 05913200	-3. 78168700	0. 02340900
C	0. 49718300	-3. 56569100	1. 88113900
C	0. 99600900	-4. 77543100	2. 39398500
C	3. 18893000	-0. 94889800	-1. 36620600
C	2. 91831900	-2. 17937900	-1. 96550200
C	2. 91204000	-2. 28264900	-3. 36439000
C	3. 28145200	-1. 20037700	-4. 15663100
C	3. 65590500	-0. 00793600	-3. 53793600
C	3. 60373400	0. 15255600	-2. 14236900
H	0. 55678600	-5. 16745700	3. 30691200
H	3. 97805400	0. 83512700	-4. 14240300
C	2. 69501400	-3. 55401600	-1. 34510000
C	4. 05686900	-4. 30249400	-1. 14613800
H	4. 51434400	-4. 59669000	-2. 09608800
H	4. 75432300	-3. 63108400	-0. 63205900
H	1. 71940600	-3. 62581700	-4. 60247500
H	3. 30302000	-4. 26043200	-4. 16512600
C	1. 07219900	-3. 05883700	0. 69788600
H	2. 43847700	-6. 36937700	2. 22440800
H	3. 28769500	-1. 27898400	-5. 24096400
C	3. 71731500	-5. 49683100	-0. 23006700
H	3. 40625900	-6. 37422700	-0. 81480000
H	4. 56675000	-5. 81448200	0. 38561400
C	2. 45915000	-3. 66150200	-3. 79427800
C	1. 87916400	-4. 24715400	-2. 48744400
H	1. 93714900	-5. 33928000	-2. 43804800
H	0. 82625300	-3. 96315900	-2. 39566900
C	4. 02166500	1. 46091900	-1. 54906000
C	5. 19705700	1. 53986100	-0. 75939700
C	3. 30512000	2. 64156200	-1. 86800600
C	5. 98873600	0. 39351800	-0. 42841600
C	5. 65515800	2. 82539700	-0. 28199700
C	3. 80052300	3. 92527100	-1. 42269300
C	7. 12002700	0. 50162700	0. 33681300
H	5. 68175700	-0. 57784100	-0. 79672600
C	6. 83859900	2. 89457700	0. 51819300
C	4. 95325400	3. 98174700	-0. 63450900
C	7. 55096600	1. 76752600	0. 82521700
H	7. 69782300	-0. 38761200	0. 57395600
H	7. 16272900	3. 87044700	0. 87273200

H	5.32290300	4.94974600	-0.30077600
H	8.44923600	1.83338500	1.43333400
C	-0.64359400	-2.92227000	2.61040600
C	-1.95367000	-2.99555900	2.07339900
C	-0.43901400	-2.38153200	3.90374200
C	-2.22958700	-3.52555900	0.77186400
C	-3.07883500	-2.54850900	2.86521000
C	-1.57342600	-1.94689200	4.68880900
C	-3.50853500	-3.59984600	0.28363900
H	-1.40321700	-3.86840400	0.16145100
C	-4.39988600	-2.65626500	2.32437400
C	-2.86028200	-2.04504800	4.15120100
C	-4.61236300	-3.16299000	1.06997200
H	-3.68344900	-3.99093400	-0.71392300
H	-5.23583300	-2.33739100	2.94379300
H	-3.71282100	-1.73236200	4.75159700
H	-5.62092600	-3.24254100	0.67289700
C	1.43896100	3.78951900	-2.95846600
H	0.51374100	3.74926200	-3.52649900
C	2.08501800	2.62812500	-2.62059900
H	1.66526200	1.67192700	-2.90762300
C	1.96157300	5.05448000	-2.56143300
H	1.44295700	5.96500500	-2.84952000
C	3.10210600	5.11504500	-1.80565300
H	3.50523900	6.07323900	-1.48444300
C	1.03125500	-1.73308000	5.74342500
H	2.03218000	-1.62287500	6.15144500
C	-0.09167500	-1.33528300	6.52429300
H	0.06093600	-0.94738000	7.52827000
C	-1.35533200	-1.43299300	6.00688000
H	-2.22112200	-1.12664600	6.59005000
C	0.86477300	-2.23511800	4.47943900
H	1.72796200	-2.49455100	3.88048000
O	1.69954600	-0.35638700	2.10570300

INT-11

0 imaginary frequencies

H = -4333.089913

G = -4333.261962

E(M06-2X-DCM) = -4333.901223

C	0.51655400	4.60478700	1.22029200
C	-0.63542100	4.19591500	2.18420700
H	-0.23117100	3.85701800	3.14201200
H	-1.27673600	5.05174400	2.40032100

C	-2.94577300	3.40044000	1.32941000
C	-3.35000900	4.70881800	1.01610700
C	-3.94374500	2.41877200	1.43669800
C	-4.69267400	5.02614700	0.82123900
H	-2.61575400	5.50002500	0.90769700
C	-5.28992500	2.73417300	1.24308300
H	-3.68648700	1.39564900	1.68356600
C	-5.67148400	4.03876500	0.93546100
H	-4.97137700	6.04741900	0.57710900
H	-6.03888000	1.95276300	1.33832000
H	-6.71922800	4.28481000	0.78695000
C	-1.47155700	3.04440800	1.54716800
C	-0.01374600	4.15417800	-0.14998300
H	0.75944400	3.97508500	-0.89937000
H	-0.74931900	4.84871100	-0.55927600
N	-0.72412300	2.86201600	0.12047000
C	-1.56654600	2.32902800	-1.00931400
N	-1.49646800	0.98454600	-0.99397800
C	-2.18671000	0.06141200	-1.80916100
C	-3.53161600	0.21841700	-2.16342000
C	-1.49007700	-1.09186000	-2.18688800
C	-4.16079900	-0.77767500	-2.90672500
C	-2.13561900	-2.07149100	-2.94012500
H	-0.45617400	-1.22160100	-1.88294600
C	-3.47007800	-1.92141000	-3.31165700
H	-3.96559500	-2.68147800	-3.90365400
C	-1.39546100	-3.33682900	-3.28103800
C	-5.63415200	-0.66823100	-3.20170900
F	-0.10000900	-3.09664000	-3.58048200
F	-1.94558300	-3.98362400	-4.32787600
F	-1.39782500	-4.20507000	-2.23455100
F	-5.94916400	-1.22580900	-4.39033000
F	-6.05605300	0.61169900	-3.22243200
F	-6.36935600	-1.31254900	-2.26050400
S	-2.37377200	3.32274700	-2.04567600
C	0.74825000	6.12443700	1.21806400
H	1.07686200	6.46471800	2.20636100
H	1.52721900	6.39899500	0.49732700
H	-0.16377800	6.67503400	0.95663100
C	1.83173600	3.88975300	1.59260000
H	2.61424900	4.10597600	0.85730900
H	2.17998600	4.24423800	2.56969500
H	1.73304300	2.80257800	1.66324400
H	-4.08095600	1.09636700	-1.85259200

C	-1.27818300	1.74173200	2.32406300
H	-0.64762600	0.59821800	-0.52192000
H	-1.79089800	1.83053300	3.28597600
H	-1.69091500	0.87050100	1.81095700
H	0.02772400	2.13284000	0.27530400
H	-0.22366600	1.53853900	2.52486000
O	0.67427400	-1.60130300	0.72877300
O	3.08018000	-0.65828600	0.49605200
P	1.57089100	-0.21887800	1.00296600
O	0.95735900	0.74246600	-0.01920200
C	1.76277600	-4.80553800	3.19540600
C	2.44533200	-4.56016300	2.00858900
C	2.01763500	-3.55092700	1.13323600
C	0.23185700	-2.96621000	2.68476700
C	0.64345600	-4.03229300	3.50259700
C	3.28070700	-1.10772000	-0.79894400
C	3.06232500	-2.45445700	-1.09617100
C	3.16170700	-2.89408600	-2.42500600
C	3.57030200	-2.02563300	-3.43222100
C	3.87921400	-0.70687300	-3.10213100
C	3.73053600	-0.21502300	-1.79363200
H	0.07989800	-4.23395700	4.40901400
H	4.22982000	-0.02569200	-3.87222700
C	2.79524800	-3.64093000	-0.17551700
C	4.12639300	-4.28472700	0.33799200
H	4.68492400	-4.78297800	-0.46095300
H	4.76327800	-3.49412700	0.75113700
H	2.10223300	-4.53995000	-3.38253400
H	3.65619400	-4.98826400	-2.68051800
C	0.97125700	-2.71016100	1.51275100
H	2.08744300	-5.59056600	3.87384800
H	3.65715200	-2.36681400	-4.46075900
C	3.68453700	-5.24141000	1.46805800
H	3.45262900	-6.24242800	1.07776200
H	4.45666700	-5.37486400	2.23454800
C	2.77187900	-4.35143400	-2.53683400
C	2.09407800	-4.62135500	-1.17676700
H	2.16584900	-5.66506000	-0.85502700
H	1.03134600	-4.36714100	-1.24274000
C	4.09218900	1.20981900	-1.51435700
C	5.22060400	1.51171200	-0.71067900
C	3.37238100	2.25653600	-2.14264500
C	6.01387800	0.50243800	-0.07631600
C	5.62762600	2.88772500	-0.53416600

C	3.81241600	3.62537100	-1.98732400
C	7.10043500	0.82554900	0.69305200
H	5.74448100	-0.53778900	-0.21347800
C	6.76539800	3.18285700	0.28056500
C	4.92080700	3.90429500	-1.18293700
C	7.48130300	2.18422300	0.88229800
H	7.68074800	0.03730100	1.16489000
H	7.05120500	4.22470400	0.40613700
H	5.24957000	4.93568400	-1.06909100
H	8.34420200	2.42112100	1.49888400
C	-0.98886200	-2.19230600	3.07404200
C	-2.17626900	-2.31655200	2.30842900
C	-0.99246800	-1.42687200	4.26622000
C	-2.24699400	-3.08219400	1.10022300
C	-3.38923400	-1.66755100	2.75671000
C	-2.22366200	-0.82525500	4.72875100
C	-3.40382700	-3.16351300	0.36950700
H	-1.36196800	-3.60489900	0.75706300
C	-4.57423800	-1.77265600	1.96033100
C	-3.38530600	-0.96009800	3.96311700
C	-4.58363200	-2.48819500	0.79296700
H	-3.41584400	-3.74647300	-0.54599300
H	-5.47354400	-1.26955500	2.30980300
H	-4.30861300	-0.50162800	4.31304500
H	-5.48147500	-2.53944800	0.18316400
C	1.54818000	3.05244300	-3.56816500
H	0.66224600	2.84670600	-4.16240700
C	2.20155900	2.02519400	-2.93674400
H	1.82754800	1.01244000	-3.02463600
C	2.01195500	4.39455800	-3.44375700
H	1.48826500	5.19492900	-3.95971300
C	3.10540900	4.66887100	-2.66629900
H	3.46485400	5.68959700	-2.55434900
C	0.15101200	-0.48229400	6.20658800
H	1.06575900	-0.31645800	6.76897400
C	-1.07310200	0.06982200	6.68128600
H	-1.08565000	0.62992600	7.61275300
C	-2.22335700	-0.09085000	5.95680600
H	-3.16172000	0.33955800	6.29967400
C	0.19143300	-1.20168400	5.04110400
H	1.13532200	-1.57908100	4.66877700
O	1.66483900	0.14848600	2.43920600

INT-11'

0 imaginary frequencies

H = -4333.082008

G = -4333.253910

E(M06-2X-DCM) = -4333.898583

O	0.51118100	2.37420600	0.42125000
O	2.56786000	0.93215700	-0.24861200
P	0.99696100	0.79931100	0.29245300
O	0.29290100	0.14802000	-0.90002300
C	0.60092100	4.90801800	-2.91718700
C	1.75632900	4.65269400	-2.18675700
C	1.70897200	3.87092700	-1.02273500
C	-0.67661300	3.50974400	-1.36291100
C	-0.60528500	4.36791100	-2.47540600
C	3.50182000	1.51737600	0.59745800
C	3.61129600	2.90892000	0.63832500
C	4.43279400	3.51228700	1.60302700
C	5.22602200	2.74125600	2.44496500
C	5.19638000	1.35493700	2.31034000
C	4.33555300	0.71415200	1.40225900
H	-1.52357700	4.59422600	-3.00913400
H	5.83687000	0.73786700	2.93370000
C	3.03766100	3.97863500	-0.28373000
C	4.00128400	4.26371600	-1.48457400
H	4.25746800	3.31076800	-1.96224100
H	4.93474000	4.73992700	-1.16865400
H	5.17335200	5.48987800	1.10587700
H	4.18183400	5.45612500	2.56004300
C	0.51891300	3.23495600	-0.66406900
H	0.62864400	5.53121500	-3.80770600
H	5.86736000	3.20633000	3.18943800
C	3.16799400	5.12753400	-2.45546800
H	3.46365400	4.99313700	-3.50265400
H	3.27772500	6.19855400	-2.23426200
C	4.29108500	5.01800400	1.56125400
C	3.03489100	5.20892600	0.68573700
H	2.13679500	5.15827700	1.31189300
H	3.01598300	6.16365800	0.15087800
C	4.40458500	-0.77787900	1.31418800
C	4.04707200	-1.56516600	2.43608800
C	4.97367400	-1.39371700	0.17076200
C	3.41115400	-1.00980200	3.59435300
C	4.31236800	-2.98617800	2.43050800
C	5.18775200	-2.82421000	0.16002400
C	3.11192100	-1.78895300	4.68189700

H	3.13376800	0.03689900	3.58365500
C	3.99458400	-3.75990000	3.59096800
C	4.86684500	-3.57738100	1.29275800
C	3.42167300	-3.17977300	4.69046200
H	2.62051000	-1.34524100	5.54342000
H	4.21516200	-4.82469700	3.57532400
H	5.05653800	-4.64893400	1.28943300
H	3.18624500	-3.77799100	5.56685200
C	-2.01192900	2.97010300	-0.96101500
C	-2.76141700	2.19276300	-1.88097600
C	-2.57847200	3.32132100	0.29181600
C	-2.24876400	1.78178800	-3.15613000
C	-4.10480600	1.77839700	-1.54369000
C	-3.90560800	2.85978500	0.63223000
C	-3.01634300	1.06857600	-4.04118800
H	-1.23207300	2.05053300	-3.41820400
C	-4.86955100	1.02772900	-2.49242100
C	-4.63545400	2.11116100	-0.29512600
C	-4.34933700	0.68955000	-3.71185600
H	-2.60455100	0.78377300	-5.00632100
H	-5.87352400	0.72055700	-2.21039600
H	-5.63623800	1.77147000	-0.03843700
H	-4.94028200	0.12112200	-4.42444200
C	5.94681400	-1.27840500	-2.07126900
H	6.26383100	-0.68869400	-2.92765400
C	5.39250300	-0.65478300	-0.98285800
H	5.27310500	0.42240300	-0.98385100
C	6.12594700	-2.69159100	-2.08786600
H	6.56803100	-3.16924400	-2.95837600
C	5.75863800	-3.43712100	-1.00006600
H	5.90627200	-4.51475200	-0.99054200
C	-2.47293800	4.45385500	2.45591900
H	-1.93328600	5.07917400	3.16196100
C	-3.76190500	3.95935300	2.80207800
H	-4.19013600	4.20018100	3.77109700
C	-4.45828600	3.19189200	1.90887600
H	-5.44975800	2.81835700	2.15255900
C	-1.90517700	4.14877200	1.24689200
H	-0.92563900	4.54103000	1.00299400
C	1.49045500	-1.83108400	-3.84032800
C	1.83876300	-2.85343800	-2.69943500
H	2.46237400	-3.67567600	-3.06159200
H	2.40418400	-2.35141700	-1.91033800
C	0.50980800	-3.82316100	-0.66224600

C	0.99453300	-2.94528800	0.31881400
C	-0.02301200	-5.05206400	-0.24149000
C	0.91058000	-3.25803200	1.67380800
H	1.42592700	-1.99033300	0.04619000
C	-0.07585000	-5.38327000	1.11328100
H	-0.40548000	-5.76702600	-0.95952100
C	0.37848800	-4.48345400	2.07587500
H	1.25350600	-2.53021300	2.40019100
H	-0.48857900	-6.34355800	1.41077800
H	0.32069200	-4.73217000	3.13179600
C	0.50892000	-3.41266600	-2.13400700
C	-0.03650600	-1.57339500	-3.66814700
H	-0.66184900	-2.12155100	-4.37288800
H	-0.30962100	-0.51719000	-3.69344400
N	-0.34427300	-2.08048000	-2.28561900
C	-1.79002900	-2.12237200	-1.86753000
N	-1.90988600	-1.46742200	-0.70320700
C	-2.99237200	-1.33023500	0.19397600
C	-4.32084400	-1.64049100	-0.10925000
C	-2.65800900	-0.81406600	1.45964600
C	-5.30659300	-1.41930600	0.85446200
C	-3.65625800	-0.62143800	2.40783100
H	-1.62563800	-0.56316900	1.69530400
C	-4.98889400	-0.92036600	2.11407500
H	-5.76442900	-0.75326700	2.85223000
C	-3.31075000	-0.12017300	3.78787600
C	-6.74834800	-1.61696200	0.47001000
F	-3.25946200	-1.14148400	4.67719200
F	-4.25183900	0.74082400	4.24323600
F	-2.12509400	0.50577500	3.82372200
F	-7.24409900	-0.50791400	-0.14515700
F	-7.53418700	-1.85007100	1.54135600
F	-6.91063500	-2.64166600	-0.39082700
S	-2.91410500	-2.90212900	-2.79437300
H	-4.58585100	-2.02162500	-1.08403500
H	-1.09787000	-0.86998100	-0.45319300
H	0.11832900	-1.36823400	-1.66282400
C	-0.02126000	-4.51941600	-3.05246600
H	-0.06597700	-4.20593600	-4.09481500
H	-1.01263000	-4.86971000	-2.77163200
H	0.68083300	-5.35701300	-2.98957200
C	2.28512700	-0.52555900	-3.64152300
H	3.36078100	-0.73255000	-3.65546300
H	2.06540400	0.18513100	-4.44791700

H	2.04791300	-0.04625100	-2.68785900
C	1.79125000	-2.38356200	-5.24581100
H	1.46917200	-1.67376300	-6.01734900
H	2.86922200	-2.53630700	-5.36889700
H	1.29407900	-3.33900600	-5.44258600
O	0.89885300	0.18725900	1.64495900

TS-PT-4

1 imaginary frequencies

H = -4333.082577

G = -4333.254037

E(M06-2X-DCM) = -4333.893064

C	-1.45727200	3.44680700	-2.58759000
C	-0.11581500	3.55061100	-3.35500700
H	-0.22293500	3.25147300	-4.40280900
H	0.22199900	4.58940900	-3.35831600
C	2.27518900	3.38691600	-2.43860800
C	2.30027800	4.68852800	-1.90922100
C	3.50362500	2.80294500	-2.78450600
C	3.49825100	5.37901400	-1.73659500
H	1.37634500	5.17345000	-1.61264400
C	4.70595600	3.49486900	-2.61831000
H	3.54091000	1.80209700	-3.19907600
C	4.70941800	4.78603500	-2.09396600
H	3.48192400	6.38147000	-1.31812900
H	5.63994900	3.01877900	-2.90501000
H	5.64416800	5.32449800	-1.96427200
C	0.94374000	2.65062500	-2.65160400
C	-0.96974100	3.19777400	-1.15159400
H	-1.70715200	2.70942200	-0.50886100
H	-0.66648400	4.12842600	-0.66588100
N	0.22602900	2.30463000	-1.27452200
C	1.08718400	2.25958700	-0.08532900
N	1.84262700	1.13652200	-0.10250900
C	2.69608600	0.72123500	0.97216200
C	4.07122500	0.69706700	0.76656700
C	2.13780900	0.27758600	2.17444100
C	4.90675500	0.21542300	1.77863200
C	2.98647500	-0.17782400	3.18167600
H	1.05866400	0.27810900	2.29145400
C	4.37015200	-0.21285100	2.99042800
H	5.02148400	-0.56967100	3.77990200
C	2.41011200	-0.71589100	4.46584600
C	6.37975900	0.07833300	1.51445700

F	3. 22192600	-0. 45936200	5. 51829300
F	2. 25396500	-2. 05991400	4. 41533900
F	1. 20261900	-0. 18535400	4. 74348400
F	7. 10845700	0. 09513800	2. 64828500
F	6. 84561800	1. 05602800	0. 70917600
F	6. 65969300	-1. 10099100	0. 88852800
S	1. 12056700	3. 40988500	1. 09747300
C	-2. 24218300	4. 76656200	-2. 67341700
H	-2. 52286300	4. 97913100	-3. 71199800
H	-3. 16486500	4. 71330000	-2. 08567900
H	-1. 64882700	5. 61227700	-2. 30509000
C	-2. 35200100	2. 30231100	-3. 10526100
H	-2. 58869600	2. 45779300	-4. 16502100
H	-1. 89312500	1. 31644700	-2. 99825500
H	-3. 29669700	2. 27667600	-2. 55131600
H	4. 48145300	1. 05524100	-0. 17100700
C	1. 12241800	1. 34790200	-3. 43823800
H	1. 56315800	0. 40212800	-0. 74785000
H	0. 16302000	0. 86167800	-3. 61456800
H	1. 57266100	1. 57328500	-4. 40939600
H	-0. 25731100	1. 07493400	-1. 34092400
H	1. 76849800	0. 62530100	-2. 93703400
O	-0. 93890100	-2. 26077800	-0. 05513500
O	-2. 86344000	-0. 56827700	-0. 43715300
P	-1. 25828100	-0. 65666900	-0. 08941200
O	-0. 88457900	-0. 07577700	1. 22129000
C	-1. 76254000	-4. 75954600	-3. 31190000
C	-2. 78428200	-4. 33936700	-2. 46701600
C	-2. 49860200	-3. 57824800	-1. 32297000
C	-0. 13510400	-3. 54847900	-1. 93966600
C	-0. 44893900	-4. 39731500	-3. 01617400
C	-3. 73581300	-1. 04590900	0. 54456900
C	-4. 03960900	-2. 40698300	0. 56913500
C	-4. 79510100	-2. 92244100	1. 63433400
C	-5. 31875800	-2. 08058700	2. 60876300
C	-5. 08029000	-0. 71027800	2. 51563400
C	-4. 27867100	-0. 16430000	1. 49972200
H	0. 36170700	-4. 75789400	-3. 64213900
H	-5. 49908900	-0. 03601700	3. 25701300
C	-3. 73885900	-3. 51598400	-0. 43476000
C	-4. 85999000	-3. 63840700	-1. 51944900
H	-5. 81085500	-3. 98296200	-1. 10114900
H	-5. 02826300	-2. 65105000	-1. 96466800
H	-4. 72855500	-4. 92011100	2. 50838500

H	-5.88128500	-4.74630000	1.18870500
C	-1.19921200	-3.11472400	-1.11899600
H	-1.97650500	-5.37397200	-4.18290300
H	-5.90462500	-2.47938300	3.43306600
C	-4.27174800	-4.59824400	-2.57756100
H	-4.51375000	-5.64548100	-2.34881900
H	-4.65508100	-4.40199800	-3.58563300
C	-4.88985000	-4.42908000	1.54199700
C	-3.79208300	-4.76481700	0.51184000
H	-3.97429600	-5.69575400	-0.03377200
H	-2.82602100	-4.85964700	1.02091900
C	-4.08425800	1.32114500	1.47326600
C	-4.79749000	2.09850500	0.52759800
C	-3.29786700	1.95295800	2.46703900
C	-5.62808300	1.51942800	-0.48617500
C	-4.72451500	3.54137600	0.58855000
C	-3.23595400	3.39682900	2.51771700
C	-6.32073700	2.29894700	-1.37661300
H	-5.71054300	0.43959500	-0.53919000
C	-5.46601600	4.31811200	-0.35736600
C	-3.94952300	4.14913400	1.58083600
C	-6.24050500	3.71969100	-1.31532900
H	-6.94429500	1.83072400	-2.13364100
H	-5.40654200	5.40226300	-0.29020400
H	-3.90581000	5.23561400	1.62887100
H	-6.80152500	4.32248800	-2.02444900
C	1.28769600	-3.15951300	-1.69170400
C	1.91932000	-3.50357500	-0.46718100
C	2.03217200	-2.50384000	-2.70893700
C	1.26403400	-4.24762000	0.56616700
C	3.29409700	-3.12120400	-0.23596700
C	3.42210100	-2.17166300	-2.47788500
C	1.89404200	-4.54068800	1.74673400
H	0.24917200	-4.58953300	0.40393400
C	3.91323900	-3.43534000	1.01518500
C	4.00671200	-2.46448600	-1.24281100
C	3.23166000	-4.11666400	1.98589600
H	1.36734900	-5.10247500	2.51316700
H	4.93740600	-3.10930500	1.17403000
H	5.04109400	-2.18185300	-1.06001600
H	3.70528100	-4.34195500	2.93703700
C	-1.78865600	1.86111300	4.38456300
H	-1.19818000	1.27996500	5.08721600
C	-2.53788500	1.21933500	3.43448100

H	-2.53066300	0.13852500	3.38005300
C	-1.74635000	3.28377000	4.44108900
H	-1.14516100	3.77368300	5.20227500
C	-2.44736200	4.02693100	3.53110800
H	-2.41453500	5.11359300	3.55639400
C	2.24178500	-1.56698800	-4.96310800
H	1.79110900	-1.31962400	-5.92071200
C	3.61690000	-1.27247700	-4.73867600
H	4.20993200	-0.82197800	-5.53014300
C	4.18041100	-1.55285600	-3.52265400
H	5.22711000	-1.32806000	-3.33044700
C	1.47685200	-2.14242800	-3.98124700
H	0.42581200	-2.32873100	-4.16475200
O	-0.60237300	-0.07327400	-1.37725300

TS-PT-4鈦?1 imaginary frequencies

H = -4333.080442

G = -4333.250448

E(M06-2X-DCM) = -4333.889867

O	-0.31045100	2.10257200	-0.64204700
O	-2.58700000	1.09767300	0.09661100
P	-0.99845000	0.71812800	-0.10893600
O	-0.55241700	0.46182500	1.35011500
C	-0.48758700	5.63370600	1.61491100
C	-1.57863400	5.21921000	0.86011600
C	-1.49024100	4.08656400	0.03571200
C	0.79658900	3.71331400	0.79687300
C	0.69595400	4.90324000	1.54121200
C	-3.37196600	1.46074200	-0.99719000
C	-3.30643900	2.76756700	-1.48272200
C	-3.97346600	3.09550500	-2.67384000
C	-4.80871100	2.17559200	-3.29644100
C	-4.97402100	0.92024800	-2.71692500
C	-4.25460700	0.52388900	-1.57457300
H	1.57173800	5.24136900	2.08633900
H	-5.66148800	0.20796700	-3.16260500
C	-2.70817200	4.03298200	-0.87855900
C	-3.76160800	4.76533300	0.02043700
H	-4.16844500	4.04618700	0.74092100
H	-4.59891300	5.16697700	-0.55831300
H	-4.50137700	5.18244500	-2.94223200
H	-3.39005500	4.57500100	-4.16423700
C	-0.34354300	3.29358400	0.08032900
H	-0.54488100	6.52250400	2.23834800

H	-5.34066500	2.43210900	-4.20908900
C	-2.95125400	5.84790000	0.76343700
H	-3.37060100	6.09021000	1.74685800
H	-2.92140800	6.78810600	0.19514900
C	-3.64693900	4.50965900	-3.10067700
C	-2.46397100	4.87171200	-2.17846400
H	-1.52287700	4.54474200	-2.63532300
H	-2.38142200	5.94373200	-1.97535800
C	-4.51865400	-0.83894400	-1.01972000
C	-4.32385600	-1.97785100	-1.84322300
C	-5.10128000	-0.98774900	0.26593900
C	-3.69962400	-1.90724100	-3.13247000
C	-4.75518400	-3.27892500	-1.38335200
C	-5.47357700	-2.30476700	0.73394000
C	-3.57342900	-3.01782400	-3.92727400
H	-3.30314500	-0.95725500	-3.46977700
C	-4.60900200	-4.41094600	-2.24561200
C	-5.30300000	-3.40907000	-0.10519900
C	-4.04878800	-4.28665500	-3.48820000
H	-3.09257400	-2.93284700	-4.89800400
H	-4.95265100	-5.37776600	-1.88562200
H	-5.61320700	-4.39258000	0.24191100
H	-3.94765900	-5.15381600	-4.13522100
C	2.11173500	3.00276100	0.77393100
C	2.69736000	2.57895700	1.99481800
C	2.83492500	2.87432000	-0.44049000
C	2.01744700	2.65407300	3.25550100
C	4.04100400	2.04637800	1.99805500
C	4.15358300	2.28207400	-0.42647600
C	2.63765200	2.29895400	4.42610000
H	0.99106100	3.00145200	3.27525700
C	4.65032500	1.68728000	3.24113300
C	4.72363200	1.89363900	0.78910300
C	3.97870900	1.82202100	4.42579100
H	2.09817100	2.37666700	5.36676500
H	5.66651900	1.30126500	3.22031700
H	5.71988800	1.45751100	0.79049700
H	4.45568900	1.54999000	5.36329800
C	-5.94944400	-0.05926400	2.36456700
H	-6.15537600	0.80308900	2.99293300
C	-5.38643100	0.12016900	1.12786800
H	-5.15858400	1.12254100	0.78670500
C	-6.27602400	-1.36300500	2.83504300
H	-6.71980900	-1.48624100	3.81935400

C	-6.04729500	-2.45058300	2.03647000
H	-6.31005700	-3.45122300	2.37185600
C	3.05643900	3.17855700	-2.85661000
H	2.64675000	3.53232500	-3.79878300
C	4.33568600	2.55495200	-2.84069300
H	4.88271100	2.42555000	-3.77025300
C	4.86946500	2.12801200	-1.65565200
H	5.84557100	1.65204300	-1.62141500
C	2.33689500	3.33610800	-1.70126800
H	1.36993000	3.82265100	-1.73876200
C	-1.20014500	-1.28058500	4.27111300
C	-1.52365500	-2.50410200	3.35073200
H	-1.95020900	-3.34286900	3.91016400
H	-2.25991900	-2.21841600	2.59504200
C	-0.35301200	-3.64843600	1.32868000
C	-1.16418500	-3.11166400	0.31934100
C	0.33652300	-4.84023000	1.04679800
C	-1.25021300	-3.71389400	-0.93513300
H	-1.71856800	-2.19563900	0.48432500
C	0.22629400	-5.46334500	-0.19645100
H	0.97288100	-5.30114700	1.79138400
C	-0.56026200	-4.89672300	-1.19714000
H	-1.84611800	-3.24417500	-1.70721500
H	0.77016800	-6.38616300	-0.38042600
H	-0.63517400	-5.36739300	-2.17354300
C	-0.20169500	-2.93456900	2.67439400
C	0.23159000	-0.85014400	3.82802900
H	1.00504700	-1.17567200	4.52463400
H	0.33700500	0.22629300	3.68524800
N	0.44422400	-1.51312900	2.49539200
C	1.82433600	-1.52767700	1.97307300
N	1.78901600	-1.47760800	0.61976700
C	2.80200200	-1.50170100	-0.36501100
C	4.16849600	-1.65980300	-0.11017700
C	2.35293600	-1.35263600	-1.69102100
C	5.06678500	-1.66279000	-1.18021700
C	3.26587100	-1.37402300	-2.73784300
H	1.29457200	-1.20552800	-1.88841000
C	4.63279200	-1.52969600	-2.49491300
H	5.33975800	-1.54931100	-3.31561600
C	2.79479000	-1.16336000	-4.15364900
C	6.54116300	-1.72817900	-0.88431700
F	1.49671800	-1.48658600	-4.31315400
F	3.51215400	-1.91100300	-5.02588700

F	2.93786200	0.12540000	-4.54015200
F	7.04925900	-0.49016700	-0.63006300
F	7.24625700	-2.22854400	-1.92066900
F	6.81176400	-2.48418700	0.19909400
S	3.14825300	-1.60662000	2.96538000
H	4.52630500	-1.77234800	0.90174700
H	0.86496200	-1.36746100	0.20032800
H	-0.18223800	-0.61322800	1.76405100
C	0.62475600	-3.78065000	3.66089000
H	0.74451500	-3.28866100	4.62436500
H	1.62415500	-4.00912200	3.29071300
H	0.09204300	-4.72114100	3.83299700
C	-2.23131600	-0.15704500	4.04497600
H	-3.23920400	-0.51606600	4.28450400
H	-2.01727300	0.70049000	4.69505100
H	-2.23165500	0.19549800	3.01132200
C	-1.21458300	-1.64376800	5.76890600
H	-0.90810500	-0.78376900	6.37686400
H	-2.22654800	-1.92477300	6.08313700
H	-0.54740700	-2.47673400	6.01208100
O	-0.72956500	-0.35199100	-1.10908400

AT-3

0 imaginary frequencies

H = -1995.965760

G = -1996.065642

E(M06-2X-DCM) = -1996.320217

C	4.17414400	0.76567600	-0.43859600
C	5.44519600	0.46732500	-1.31008600
H	5.47465400	1.18077600	-2.14486700
H	6.32412000	0.67833500	-0.68500700
C	5.54687100	-0.93464200	-1.84625100
C	2.95006200	0.52571100	-1.35905400
H	2.91813900	-0.50493900	-1.71328300
H	3.07245800	1.15449500	-2.25336700
N	1.66709400	0.81919300	-0.73438100
C	0.51358800	0.13026800	-0.92413600
N	-0.55567800	0.74770000	-0.29237900
C	-1.90299700	0.35685000	-0.17718400
C	-2.31692200	-0.97798900	-0.06751000
C	-2.85902500	1.37759200	-0.08906000
C	-3.67038200	-1.26540300	0.10496500
C	-4.20550800	1.07286900	0.09949700
H	-2.55160600	2.41674000	-0.16389800

C	-4.62591800	-0.25268400	0.19151200
H	-5.67117200	-0.49075000	0.34585100
C	-5.21725400	2.18789500	0.13865300
C	-4.11165700	-2.70634800	0.16737900
F	-5.66280300	2.50034100	-1.09923900
F	-4.69346000	3.32013300	0.66322300
F	-6.29800900	1.85908600	0.87683700
F	-5.22960000	-2.85226500	0.91383100
F	-3.16010600	-3.50135500	0.70096300
F	-4.39229400	-3.19195000	-1.06173100
S	0.40424900	-1.28507700	-1.82355900
C	4.26656900	2.28207400	-0.05131100
H	4.19194500	2.87672700	-0.97110700
H	5.27541400	2.46864000	0.34265700
H	-1.59033400	-1.77593000	-0.11198200
C	5.63530500	-1.24635100	-3.14025400
H	-0.39273500	1.70640200	-0.00684100
H	5.72119100	-2.27646800	-3.47497700
H	1.64613000	1.64727800	-0.14770900
C	4.19146000	-0.13976300	0.80577600
C	3.33562500	-1.24252200	0.94983300
C	5.13224800	0.08977200	1.82582200
C	3.41169400	-2.07260600	2.07147600
H	2.59927800	-1.47502300	0.18816600
C	5.20888300	-0.73618700	2.94662500
H	5.82535400	0.92340600	1.74990700
C	4.34428800	-1.82392800	3.07667300
H	2.73359300	-2.91805100	2.15195400
H	5.94784300	-0.52892100	3.71634500
H	4.40026000	-2.46969200	3.94876000
C	3.27872500	2.79948300	0.96340000
C	2.47806600	3.85612700	0.78311300
H	2.47577800	4.42250200	-0.14680100
H	5.62819000	-0.48361900	-3.91681400
H	1.81919400	4.21347500	1.57065200
H	5.55672500	-1.73210200	-1.10401000
H	3.25575600	2.27449100	1.91798500

AT-3-1

0 imaginary frequencies

H = -1995.963958

G = -1996.064069

E(M06-2X-DCM) = -1996.319612

0 1

C	-4.13045300	0.80502800	0.57980100
C	-5.39628600	0.50209300	1.46237900
H	-5.39546800	1.21724200	2.29928300
H	-6.28454300	0.72452600	0.86044600
C	-5.50710500	-0.89671600	2.00809600
C	-2.89141200	0.51597400	1.46464600
H	-2.85410400	-0.53112500	1.76522700
H	-2.98835000	1.10457400	2.38931800
N	-1.61823500	0.82175200	0.82721400
C	-0.46541800	0.12546400	0.99162600
N	0.59638300	0.73903900	0.34506800
C	1.94069500	0.34216100	0.21293900
C	2.34458100	-0.99399800	0.08533600
C	2.90312100	1.35760000	0.13535200
C	3.69594500	-1.28891000	-0.09094900
C	4.24697900	1.04566900	-0.06072800
H	2.60533600	2.39671300	0.24178300
C	4.65812400	-0.28162800	-0.16719500
H	5.70355600	-0.52570300	-0.31065300
C	5.24992100	2.15855100	-0.21390000
C	4.12886900	-2.73204800	-0.15941700
F	6.48138600	1.78500700	0.19046800
F	4.89835800	3.25241000	0.49972300
F	5.35920700	2.55293700	-1.50420300
F	5.24594500	-2.88116400	-0.90654600
F	3.17248800	-3.51869800	-0.69648600
F	4.40675900	-3.22465100	1.06752500
S	-0.35019500	-1.29529300	1.88266500
C	-4.20377200	2.33607200	0.24658200
H	-4.09209800	2.89769100	1.18327500
H	-5.21964200	2.55401600	-0.11143000
H	1.61296000	-1.78763300	0.12489800
C	-6.41979900	-1.78784700	1.61965200
H	0.43268400	1.69770000	0.05979000
H	-6.46503500	-2.78398600	2.05128000
H	-1.60517500	1.65743800	0.25118400
C	-4.18580900	-0.05694500	-0.69248600
C	-3.35480500	-1.16953400	-0.88875300
C	-5.13679700	0.22676000	-1.68854000
C	-3.46325900	-1.95724300	-2.03752500
H	-2.61172200	-1.44365500	-0.14791800
C	-5.24719500	-0.55730500	-2.83633900
H	-5.81210000	1.07046500	-1.57253400
C	-4.40595500	-1.65570800	-3.01843200

H	-2.80338100	-2.81226900	-2.15833900
H	-5.99344700	-0.30854100	-3.58656500
H	-4.48752500	-2.26892300	-3.91177700
C	-3.23627000	2.87086500	-0.77885900
C	-2.41073700	3.90603400	-0.58610100
H	-2.37008200	4.43906500	0.36246900
H	-7.15526600	-1.55655300	0.85189800
H	-1.76902400	4.27924200	-1.38043500
H	-4.79597700	-1.17969000	2.78404200
H	-3.25177400	2.37963900	-1.75129100

AT-3-2

0 imaginary frequencies

H = -1995.962103

G = -1996.062812

E(M06-2X-DCM) = -1996.316907

C	3.96784100	0.54940700	-0.32080600
C	4.05085100	1.19500100	-1.75244800
H	5.01404800	1.71607500	-1.82240400
H	4.09103500	0.38370300	-2.49039200
C	2.98556600	2.18593600	-2.15164900
C	2.79600400	-0.46112900	-0.23931800
H	2.80004400	-0.96143800	0.73007700
H	2.91966200	-1.23788300	-1.00671300
N	1.48668900	0.16318000	-0.38634200
C	0.32525500	-0.42457100	0.01987000
N	-0.76773000	0.37579200	-0.28857300
C	-2.14569900	0.14195300	-0.13111100
C	-2.73639000	-1.12236800	-0.26922300
C	-2.96271900	1.25430300	0.11029500
C	-4.11836600	-1.25195700	-0.14473400
C	-4.34461100	1.10826200	0.21841700
H	-2.51803600	2.23768300	0.23327800
C	-4.93586900	-0.14756400	0.10019300
H	-6.00714900	-0.26606300	0.20755900
C	-5.20292900	2.32956000	0.41785600
C	-4.75382400	-2.60393000	-0.35283400
F	-5.54801200	2.89051600	-0.76487600
F	-4.56035000	3.28413600	1.12883300
F	-6.34916700	2.03888200	1.06660900
F	-3.91936200	-3.61210700	-0.03192300
F	-5.11401100	-2.78241000	-1.64599200
F	-5.87464400	-2.74592400	0.38868200
S	0.24657100	-1.89370400	0.81828700

C	3.78245900	1.65770900	0.76646000
H	2.82052500	2.15626700	0.60750400
H	4.55908700	2.42100500	0.61593500
H	-2.12175000	-1.99121500	-0.45459500
C	2.17905500	2.06105300	-3.21146900
H	-0.54112600	1.34827600	-0.46156600
H	1.46708500	2.83597000	-3.48421700
H	1.41781500	0.85599000	-1.12603700
C	5.30482600	-0.19389000	-0.09057700
C	5.39357900	-1.58220100	0.09003100
C	6.50612500	0.53726700	-0.05904800
C	6.62641400	-2.21116800	0.28711700
H	4.50399200	-2.20110400	0.08582300
C	7.73664800	-0.08503900	0.14020300
H	6.48836200	1.61650800	-0.18571800
C	7.80411000	-1.46867500	0.31252400
H	6.65667700	-3.28891000	0.42342800
H	8.64326900	0.51403600	0.16135500
H	8.76165900	-1.95829700	0.46686700
C	3.84286600	1.15927500	2.18621000
C	2.83675100	1.23400400	3.05838500
H	1.87410700	1.66451800	2.79010300
H	2.21924400	1.18842900	-3.86082000
H	2.93313300	0.86280000	4.07497700
H	2.91696800	3.09257300	-1.54937700
H	4.78576900	0.71227200	2.49867200

AT-3-3

0 imaginary frequencies

H = -1995.960250

G = -1996.060119

E(M06-2X-DCM) = -1996.316409

C	-3.77022800	-0.68391800	0.02606700
C	-4.24743800	-2.09528100	0.49818600
H	-4.86429700	-1.96945400	1.39429400
H	-4.89163500	-2.51583400	-0.28406200
C	-3.17046400	-3.11432000	0.78234400
C	-2.74722300	-0.83185000	-1.15101300
H	-2.67405000	0.09380700	-1.71757900
H	-3.10901600	-1.60681400	-1.83941800
N	-1.38330400	-1.16039100	-0.75185700
C	-0.31034800	-0.32594500	-0.84486400
N	0.84299800	-0.94125900	-0.38074500
C	2.14737900	-0.42679600	-0.23906300

C	2.41136800	0.87926600	0.19561500
C	3.21562300	-1.30294700	-0.46417400
C	3.73108800	1.28932500	0.37545500
C	4.52951700	-0.88169700	-0.26369200
H	3.02405700	-2.32010200	-0.79364700
C	4.80005000	0.42025100	0.15140600
H	5.81995200	0.74607700	0.31520000
C	5.66203100	-1.82914600	-0.56178000
C	4.01081300	2.71198600	0.79122200
F	6.75804500	-1.54813300	0.17326700
F	6.02986100	-1.77219900	-1.86146700
F	5.31779600	-3.11307700	-0.30820200
F	5.14015200	2.80006100	1.52929000
F	3.00337100	3.22921400	1.52550900
F	4.17688600	3.51706900	-0.28076500
S	-0.36396000	1.22742500	-1.47800700
C	-3.10052900	0.07484800	1.21802700
H	-2.65700300	0.99895100	0.82449800
H	-2.26970600	-0.52541700	1.60390800
H	1.59679700	1.56023700	0.39547600
C	-2.73287000	-3.46977700	1.99380600
H	0.80434500	-1.95350900	-0.34741700
H	-1.97760600	-4.24030600	2.12721900
H	-1.28346200	-1.97990200	-0.16351000
C	-4.95860600	0.15084100	-0.50485300
C	-4.71715800	1.43309800	-1.03357100
C	-6.29030900	-0.28593000	-0.45803000
C	-5.75611500	2.23279200	-1.50529600
H	-3.70260800	1.82041600	-1.07882600
C	-7.33489600	0.51386100	-0.93085300
H	-6.53904700	-1.25599600	-0.04332000
C	-7.07443100	1.77542500	-1.45980900
H	-5.53185500	3.21634500	-1.90956400
H	-8.35509000	0.14217600	-0.88028000
H	-7.88593500	2.39657400	-1.82900300
C	-4.02992100	0.41509500	2.35230800
C	-3.84004700	0.05936700	3.62467200
H	-2.97705900	-0.52775600	3.93403100
H	-3.12940500	-3.01389100	2.89806500
H	-4.52946400	0.35652700	4.41060100
H	-2.75754500	-3.63065300	-0.08799400
H	-4.90358900	1.01357600	2.09632600

0 imaginary frequencies

H = -1995.960049

G = -1996.059913

E(M06-2X-DCM) = -1996.316346

C	-4.15619100	-0.74841200	-0.59349400
C	-5.41077800	-0.32013300	-1.44231600
H	-5.41813900	-0.89937600	-2.37551000
H	-6.30243600	-0.62331900	-0.87617700
C	-5.50810000	1.14604500	-1.76427200
C	-2.92153900	-0.36416500	-1.44799200
H	-2.89649400	0.70862100	-1.64161200
H	-3.02843400	-0.84854700	-2.42983800
N	-1.64243300	-0.74000100	-0.86150200
C	-0.48475500	-0.04256100	-0.97909900
N	0.57672600	-0.71804900	-0.39434100
C	1.92628100	-0.34819700	-0.24341900
C	2.34844600	0.96932400	-0.01761500
C	2.87667700	-1.37805100	-0.25146000
C	3.70474000	1.23335400	0.16956600
C	4.22576400	-1.09837700	-0.04339600
H	2.56506200	-2.40240700	-0.43418400
C	4.65471600	0.21177200	0.16074300
H	5.70419900	0.43146700	0.31372200
C	5.21556600	-2.23170900	0.01623400
C	4.15639900	2.66165200	0.34436700
F	6.44807800	-1.84404200	-0.37155300
F	4.84361700	-3.26500200	-0.77328200
F	5.33179500	-2.72264300	1.27243100
F	4.43174300	3.24340600	-0.84350800
F	5.28069400	2.73981000	1.09162200
F	3.21407700	3.41662100	0.94782800
S	-0.36389300	1.44509000	-1.75074500
C	-4.26491300	-2.30232500	-0.46642700
H	-4.17635900	-2.70795300	-1.48457300
H	-5.29266700	-2.55972400	-0.16790700
H	1.62685300	1.77256100	0.00883200
C	-5.57039700	1.64711400	-2.99899100
H	0.40625900	-1.69673100	-0.19390900
H	-5.65627300	2.71535200	-3.17800500
H	-1.64039800	-1.59769100	-0.31929600
C	-4.21965300	-0.02598600	0.76253600
C	-3.39115500	1.06255200	1.07663400
C	-5.18235600	-0.40798500	1.71296300
C	-3.51378100	1.73179300	2.29778900

H	-2.63830400	1.40535100	0.37474000
C	-5.30739500	0.25893500	2.93035600
H	-5.84556000	-1.24390900	1.50772600
C	-4.46946900	1.33434700	3.23096000
H	-2.85532100	2.56933100	2.51233800
H	-6.06031700	-0.06422700	3.64455000
H	-4.56260500	1.85529600	4.17995300
C	-3.34756300	-3.11634700	0.42507200
C	-2.61821400	-2.75149200	1.48596200
H	-2.58039400	-1.73330900	1.85846300
H	-5.54050500	1.00917000	-3.88043300
H	-2.04782300	-3.49412800	2.03878600
H	-5.54081200	1.82376200	-0.91201300
H	-3.34134800	-4.17492000	0.15714700

AT-4

0 imaginary frequencies

H = -2074.545648

G = -2074.653087

E(M06-2X-DCM) = -2074.938512

C	-3.94624100	0.72531700	0.42906800
C	-5.26551800	0.24020900	1.12982000
H	-5.31206700	0.68903000	2.13164500
H	-6.10622700	0.66030500	0.55986100
C	-5.43285500	-1.25052900	1.23982500
C	-2.77508600	0.18878500	1.28942500
H	-2.78936000	-0.90010400	1.34075400
H	-2.91973400	0.54721100	2.31933400
N	-1.45802300	0.59526100	0.81697700
C	-0.33069600	-0.15607900	0.86331700
N	0.77840700	0.56351700	0.44174700
C	2.11976700	0.17015300	0.28069000
C	2.50751600	-1.10828900	-0.14440400
C	3.10272900	1.14616700	0.49313300
C	3.86098100	-1.39134000	-0.32362300
C	4.44945200	0.85142900	0.29045200
H	2.81784800	2.13818500	0.83156000
C	4.84314000	-0.42338300	-0.11189200
H	5.89029000	-0.65636700	-0.26126000
C	5.47741700	1.93945700	0.45453500
C	4.27282600	-2.78819000	-0.71575800
F	5.66249300	2.62462300	-0.69828500
F	6.67920000	1.44589700	0.81748300
F	5.10646400	2.84361300	1.38979600

F	4.48789500	-3.56448000	0.36895800
F	5.41984600	-2.78565100	-1.43204800
F	3.32918100	-3.40020600	-1.46194400
S	-0.29065500	-1.75470100	1.38160900
C	-3.98045900	2.29157400	0.48296000
H	-3.93676700	2.59675500	1.53684400
H	-4.96623500	2.61753700	0.12215600
H	1.76136200	-1.86704300	-0.32911200
C	-5.55854200	-1.91900600	2.39042400
H	0.64894800	1.56766500	0.39826600
H	-1.40037400	1.54302700	0.45656000
C	-3.92536100	0.20726000	-1.01968800
C	-4.80299600	0.75497300	-1.97253400
C	-3.09843500	-0.84860000	-1.43317700
C	-4.84633000	0.27996500	-3.28281700
H	-5.47211800	1.56454700	-1.69366400
C	-3.14083200	-1.32732100	-2.74535700
H	-2.41137400	-1.31795700	-0.73748100
C	-4.01072500	-0.76557300	-3.67801200
H	-5.53674400	0.72749500	-3.99321200
H	-2.48621600	-2.14602000	-3.03244800
H	-4.04066400	-1.13815100	-4.69833800
C	-2.93132400	3.04017800	-0.30119900
C	-2.12224700	3.98214300	0.20343600
H	-2.19155100	4.21930000	1.26755700
H	-5.53045300	-1.36088500	3.32887700
H	-5.45962400	-1.80392600	0.30071600
H	-2.87360100	2.81241400	-1.36627600
C	-5.74350400	-3.40400600	2.51371400
H	-5.76123100	-3.89012300	1.53267100
H	-4.93377100	-3.85561200	3.10215600
H	-6.68151600	-3.64636900	3.03157900
C	-1.13247800	4.78937600	-0.58949700
H	-0.11734100	4.70719100	-0.17709100
H	-1.10301000	4.47626400	-1.63841200
H	-1.38759100	5.85723800	-0.56273800

AT-4-1

0 imaginary frequencies

H = -2074.544259

G = -2074.651909

E(M06-2X-DCM) = -2074.936929

C	-3.91318600	-0.09747300	0.08051900
C	-5.17538600	-0.62133700	0.86397400

H	-6.00046200	-0.69643400	0.14591000
H	-4.95123100	-1.64820500	1.18432200
C	-5.62416800	0.18783700	2.05342200
C	-2.74287800	-0.03856200	1.09591300
H	-2.59944400	-0.99987400	1.59257000
H	-2.99995000	0.68508200	1.87997600
N	-1.46532200	0.33782700	0.50427000
C	-0.25247100	-0.15507000	0.85407900
N	0.77509700	0.49498800	0.18696600
C	2.16550600	0.27759200	0.21131300
C	2.74961300	-0.99068000	0.33543800
C	2.99118600	1.39489700	0.02829600
C	4.13805000	-1.11368500	0.29963800
C	4.37617600	1.25108800	-0.02471900
H	2.55278400	2.38473300	-0.05992000
C	4.96423400	-0.00409400	0.11915500
H	6.04103800	-0.11611600	0.08705000
C	5.23512900	2.45781700	-0.29590400
C	4.75962400	-2.47290700	0.50165700
F	5.40535500	2.65688300	-1.62403700
F	6.46440800	2.33234900	0.24513900
F	4.68268500	3.58864900	0.19989800
F	5.94587100	-2.57729900	-0.13907000
F	3.96316200	-3.46286200	0.04622100
F	4.99496400	-2.72088900	1.80876900
S	-0.03161800	-1.39289700	1.97129000
C	-4.23483900	1.33808000	-0.45057100
H	-4.37320100	1.99700000	0.41412200
H	-5.21461400	1.30391500	-0.94744900
H	2.12658300	-1.86424600	0.45927800
C	-6.76910600	0.87580200	2.11672700
H	0.51483000	1.36474400	-0.26330300
H	-1.51648300	1.07744900	-0.18984700
C	-3.66076800	-1.09858800	-1.06171800
C	-4.45334800	-1.06476300	-2.22234100
C	-2.70786800	-2.12444300	-0.95938300
C	-4.29438600	-2.00271000	-3.24245500
H	-5.21509200	-0.29919800	-2.33960900
C	-2.54728800	-3.06557900	-1.97893300
H	-2.07341300	-2.20658900	-0.08315200
C	-3.33596100	-3.00978100	-3.12688600
H	-4.92394500	-1.94478300	-4.12674300
H	-1.79766600	-3.84468300	-1.86815600
H	-3.20800400	-3.74161300	-3.91986800

C	-3.24616300	1.95680900	-1.40767700
C	-2.65112800	3.14513200	-1.23347100
H	-2.86351100	3.71016700	-0.32313900
H	-7.43083200	0.87260100	1.24786200
H	-4.97717600	0.17790500	2.93196000
H	-3.04467100	1.39876900	-2.32318400
C	-7.24796800	1.65744200	3.30625300
H	-7.40683700	2.71405600	3.05124200
H	-8.21170300	1.27593000	3.66970100
H	-6.53212200	1.61169800	4.13386800
C	-1.72581800	3.80396700	-2.21827700
H	-1.54327400	3.16744900	-3.09059800
H	-2.14614500	4.75355700	-2.57572700
H	-0.75672600	4.05111000	-1.76302100

AT-4-2

0 imaginary frequencies

H = -2074.544173

G = -2074.652075

E(M06-2X-DCM) = -2074.936832

C	3.91449900	0.09515700	0.08503600
C	5.17471200	0.60790300	0.87894100
H	6.00266900	0.68926500	0.16487900
H	4.95130000	1.63163000	1.20969100
C	5.61739800	-0.21507400	2.06119000
C	2.74031400	0.02685700	1.09537800
H	2.59708100	0.98262000	1.60268400
H	2.99293000	-0.70639000	1.87193800
N	1.46427700	-0.33979700	0.49452200
C	0.25095500	0.15091900	0.84629400
N	-0.77508700	-0.48838100	0.16699300
C	-2.16570400	-0.27206000	0.18771600
C	-2.75322000	0.99138900	0.34133600
C	-2.98788600	-1.38419300	-0.03871700
C	-4.14122300	1.11440300	0.28790700
C	-4.37205300	-1.24050000	-0.10542100
H	-2.54608000	-2.36806600	-0.16777100
C	-4.96357400	0.01005200	0.06424700
H	-6.03894900	0.12468200	0.00481100
C	-5.23427700	-2.46023000	-0.29800700
C	-4.76603800	2.46935300	0.50867500
F	-4.60350400	-3.40868100	-1.02892200
F	-6.39031900	-2.16291700	-0.92756600
F	-5.56198800	-3.03077000	0.88339300

F	-3.96433300	3.46861000	0.08367900
F	-5.01815900	2.69094900	1.81740900
F	-5.94388300	2.58631200	-0.14509000
S	0.02925000	1.37454800	1.97897900
C	4.23558600	-1.33486300	-0.46108600
H	4.36994900	-2.00363200	0.39664600
H	5.21706800	-1.29680000	-0.95430200
H	-2.13279300	1.86201400	0.49517500
C	6.76076700	-0.90592100	2.12136100
H	-0.51304100	-1.34992700	-0.29782000
H	1.51669100	-1.07184400	-0.20748000
C	3.66797400	1.10965000	-1.04664000
C	4.46404500	1.08712000	-2.20514300
C	2.71713000	2.13651700	-0.93562900
C	4.31038600	2.03692300	-3.21505600
H	5.22440000	0.32117600	-2.32875500
C	2.56183300	3.08949000	-1.94494700
H	2.08016800	2.21024800	-0.06046700
C	3.35391800	3.04484400	-3.09104200
H	4.94255300	1.98754800	-4.09800200
H	1.81364500	3.86901500	-1.82764500
H	3.23008800	3.78588800	-3.87608600
C	3.24903600	-1.94116300	-1.42829500
C	2.65093200	-3.13005100	-1.26906200
H	2.85897400	-3.70537100	-0.36419200
H	7.42580600	-0.89457600	1.25509600
H	4.96706800	-0.21339600	2.93731500
H	3.05181500	-1.37279300	-2.33836100
C	7.23360200	-1.70131800	3.30415600
H	8.19666800	-1.32563000	3.67536100
H	6.51469400	-1.66313500	4.12949600
H	7.39143400	-2.75542000	3.03833300
C	1.72759600	-3.77613600	-2.26411100
H	0.75647700	-4.02626400	-1.81484600
H	1.54930300	-3.12970500	-3.13000700
H	2.14718800	-4.72261100	-2.63057400

AT-4-3

0 imaginary frequencies

H = -2074.544175

G = -2074.652066

E(M06-2X-DCM) = -2074.936830

C	3.91438000	-0.09531400	-0.08507900
C	5.17477500	-0.60803800	-0.87877600

H	6.00258900	-0.68939200	-0.16455000
H	4.95142500	-1.63176200	-1.20957100
C	5.61768500	0.21499200	-2.06090000
C	2.74038900	-0.02718900	-1.09564000
H	2.59711200	-0.98309100	-1.60268100
H	2.99324400	0.70578900	-1.87237000
N	1.46426800	0.33984100	-0.49513600
C	0.25095200	-0.15081100	-0.84699900
N	-0.77513000	0.48878700	-0.16807600
C	-2.16571200	0.27226200	-0.18839000
C	-2.75314700	-0.99129100	-0.34175800
C	-2.98797100	1.38428900	0.03816300
C	-4.14109100	-1.11445700	-0.28790700
C	-4.37213200	1.24043900	0.10527000
H	-2.54624500	2.36823300	0.16704000
C	-4.96354300	-0.01016800	-0.06410800
H	-6.03888600	-0.12492200	-0.00437300
C	-5.23412900	2.46029600	0.29805600
C	-4.76598500	-2.46941600	-0.50838600
F	-5.55808000	3.03362900	-0.88304200
F	-4.60463800	3.40674900	1.03270100
F	-6.39208700	2.16252100	0.92379900
F	-5.94253200	-2.58704600	0.14762300
F	-3.96326500	-3.46880200	-0.08568400
F	-5.02069500	-2.69011200	-1.81678700
S	0.02928600	-1.37458000	-1.97956700
C	4.23529900	1.33476000	0.46101700
H	4.36950600	2.00357600	-0.39670500
H	5.21683400	1.29680900	0.95413500
H	-2.13267000	-1.86184700	-0.49577300
C	6.76107500	0.90584100	-2.12077200
H	-0.51305900	1.35033900	0.29671000
H	1.51669500	1.07167400	0.20708600
C	3.66777300	-1.10969700	1.04666800
C	4.46402800	-1.08732600	2.20503900
C	2.71658800	-2.13629100	0.93587300
C	4.31024800	-2.03703300	3.21503500
H	5.22462400	-0.32159200	2.32849700
C	2.56117600	-3.08916100	1.94526300
H	2.07947600	-2.20985300	0.06080700
C	3.35347000	-3.04468200	3.09123000
H	4.94257000	-1.98777600	4.09787800
H	1.81275000	-3.86848600	1.82813400
H	3.22955500	-3.78565800	3.87632600

C	3.24877000	1.94092500	1.42834100
C	2.65077500	3.12989800	1.26932300
H	2.85885700	3.70536200	0.36455200
H	7.42593200	0.89441900	-1.25436700
H	4.96755600	0.21337900	-2.93717400
H	3.05149200	1.37242500	2.33831300
C	7.23417800	1.70135800	-3.30338300
H	8.19740200	1.32580900	-3.67431900
H	6.51552600	1.66315500	-4.12894700
H	7.39180400	2.75546200	-3.03743800
C	1.72752200	3.77590700	2.26450700
H	1.54919400	3.12935200	3.13030600
H	2.14721400	4.72228300	2.63111400
H	0.75641100	4.02619000	1.81531100

AT-5

0 imaginary frequencies

H = -2074.531282

G = -2074.637582

E(M06-2X-DCM) = -2074.934353

C	3.65053100	0.47442500	-0.48209300
C	3.63916700	0.26376800	-2.04309600
H	2.77563100	0.80122500	-2.46416000
H	4.51285600	0.78285800	-2.44847800
C	3.62666600	-1.17021800	-2.55695600
C	2.47927600	-0.28324000	0.18062500
H	2.49989800	-0.13904800	1.26231700
H	2.57712000	-1.36084300	0.00358000
N	1.17754900	0.17402500	-0.29804100
C	-0.00691300	-0.21115800	0.25517600
N	-1.08556300	0.35916400	-0.40909500
C	-2.46612600	0.16757300	-0.20610800
C	-3.02513100	-1.07935700	0.10524600
C	-3.31019500	1.26709700	-0.40282200
C	-4.40754200	-1.19861900	0.23586100
C	-4.69233600	1.12600700	-0.28718300
H	-2.88929000	2.24113100	-0.63498100
C	-5.25374800	-0.10594700	0.04127900
H	-6.32690900	-0.21443600	0.13968800
C	-5.58226500	2.30617500	-0.57676200
C	-4.99696400	-2.52792800	0.63653700
F	-4.98728700	3.47483900	-0.24666400
F	-6.74756400	2.23490500	0.09840000
F	-5.88986900	2.38245200	-1.89266700

F	-5.09886900	-2.63996900	1.97873400
F	-4.24279800	-3.56165400	0.20668500
F	-6.24002300	-2.69224300	0.13111800
S	-0.11288400	-1.20955500	1.59304900
C	3.52250900	2.02143300	-0.22795000
H	2.62924000	2.37843600	-0.75757100
H	4.37253700	2.50436100	-0.72073800
H	-2.38887000	-1.94168700	0.24289900
C	4.75721500	-1.86817800	-2.71039300
H	-0.86703000	1.20186100	-0.92814500
H	4.74483700	-2.88933900	-3.08359500
H	1.14688900	0.54474400	-1.23933600
C	4.98989300	-0.03703800	0.08802900
C	6.19830600	0.50843900	-0.38159200
C	5.07648300	-1.03188300	1.07116600
C	7.43267300	0.08179000	0.10406900
H	6.18519600	1.28545700	-1.14126000
C	6.31198500	-1.46431500	1.56195000
H	4.18261900	-1.49166100	1.47651000
C	7.49663100	-0.91217200	1.08267300
H	8.34489700	0.52815600	-0.28335600
H	6.33889800	-2.23820700	2.32444200
H	8.45671600	-1.24838100	1.46436000
C	3.45374600	2.49214400	1.21916300
C	4.56275500	2.73365400	1.92710900
H	5.55635900	2.58619700	1.51448300
H	5.73001000	-1.45432700	-2.46274600
H	4.51209500	3.08053400	2.95638000
C	2.28843500	-1.76027300	-2.94128800
H	1.79964100	-1.15077400	-3.71520800
H	2.39987200	-2.77393200	-3.33746800
H	1.59368600	-1.81046800	-2.09347400
C	2.08427900	2.73841500	1.81081800
H	1.52144400	3.46088000	1.20261800
H	1.47608500	1.82743400	1.85805500
H	2.15951500	3.14184500	2.82516600

AT-5-1

0 imaginary frequencies

H = -2074.534410

G = -2074.639542

E(M06-2X-DCM) = -2074.933667

C	3.54221800	0.54127900	0.07841900
C	3.47591000	1.95233800	-0.61702700

H	2. 62784000	2. 49365000	-0. 18066100
H	4. 37102500	2. 51236700	-0. 32022400
C	3. 34993300	2. 01165900	-2. 12890300
C	2. 44097400	-0. 37736900	-0. 52354300
H	2. 34742500	-1. 30947100	0. 03196400
H	2. 70081500	-0. 63373300	-1. 55780000
N	1. 12092100	0. 24485900	-0. 53374800
C	-0. 04511700	-0. 36753800	-0. 17093900
N	-1. 12934900	0. 46824200	-0. 39803000
C	-2. 50689800	0. 22793700	-0. 22556500
C	-3. 11354900	-0. 99692600	-0. 53486700
C	-3. 30222100	1. 29792000	0. 20188300
C	-4. 49262900	-1. 13631200	-0. 38911700
C	-4. 68283600	1. 14722000	0. 32387700
H	-2. 84327500	2. 24958300	0. 45362400
C	-5. 29013400	-0. 07349600	0. 03774700
H	-6. 36164000	-0. 19395400	0. 14048400
C	-5. 52444300	2. 33377600	0. 71408900
C	-5. 12963200	-2. 47636600	-0. 65983000
F	-6. 65646500	1. 96138800	1. 34572900
F	-5. 89390200	3. 05592700	-0. 36948600
F	-4. 85465400	3. 17505500	1. 53398500
F	-6. 40200800	-2. 34208800	-1. 09661800
F	-5. 17372700	-3. 23806000	0. 45487500
F	-4. 45051200	-3. 17585900	-1. 59342300
S	-0. 15434600	-1. 89979500	0. 49611100
C	3. 25457700	0. 82312700	1. 60234800
H	2. 16487100	0. 93926200	1. 69582900
H	3. 68432100	1. 80119400	1. 84740400
H	-2. 51606400	-1. 82642900	-0. 88439700
C	2. 29199300	2. 60994300	-2. 69675900
H	-0. 89760900	1. 45182900	-0. 47648800
H	2. 19236000	2. 69966600	-3. 77541100
H	1. 03793700	1. 00313800	-1. 20374500
C	4. 93501000	-0. 09205300	-0. 09663900
C	6. 07620500	0. 61406700	0. 32240600
C	5. 13482100	-1. 37366300	-0. 63304300
C	7. 35567700	0. 07883200	0. 19175400
H	5. 96869300	1. 59719000	0. 77153400
C	6. 41679400	-1. 91566500	-0. 76572400
H	4. 29282100	-1. 97492500	-0. 95807500
C	7. 53455500	-1. 19139200	-0. 35924500
H	8. 21432400	0. 65467800	0. 52711500
H	6. 53327300	-2. 91006900	-1. 18857800

H	8.53127300	-1.61118300	-0.46319900
C	3.74073600	-0.16426700	2.64740700
C	4.56874100	0.24509400	3.61562200
H	4.94509300	1.26447200	3.66027500
H	1.50754400	3.07680300	-2.10220500
H	4.89967500	-0.42609500	4.40427900
C	4.47310800	1.45705500	-2.97134400
H	4.29469900	1.63588700	-4.03599200
H	5.42688900	1.92612800	-2.69734800
H	4.61224900	0.38149400	-2.81920200
C	3.22761600	-1.58276300	2.61185600
H	3.51971100	-2.12744400	3.51506900
H	2.13496000	-1.61811400	2.52299500
H	3.63226300	-2.13282900	1.75268500

AT-5-2

0 imaginary frequencies

H = -2074.533739

G = -2074.640430

E(M06-2X-DCM) = -2074.933959

C	3.77253700	0.55831700	0.09438400
C	3.84347700	2.05467500	-0.41797300
H	4.63742400	2.54826000	0.15197600
H	4.19363600	2.01518000	-1.45588100
C	2.59979900	2.93424100	-0.37111000
C	2.58641100	-0.21096900	-0.53259600
H	2.64904200	-1.26977300	-0.26824600
H	2.63083000	-0.15241000	-1.62746500
N	1.28982600	0.27576900	-0.07951700
C	0.11290500	-0.32635500	-0.38223200
N	-0.97142100	0.37244500	0.12869800
C	-2.35273100	0.11519200	0.05308500
C	-2.90582100	-1.17250100	0.01207300
C	-3.20911700	1.22433900	0.09874700
C	-4.29222500	-1.32364200	-0.00360500
C	-4.59147000	1.05363900	0.09814600
H	-2.79550200	2.22798400	0.13976200
C	-5.14787400	-0.22309200	0.04018800
H	-6.22251800	-0.35791600	0.04789200
C	-5.48655300	2.26485400	0.09429200
C	-4.87664400	-2.71071500	-0.10363500
F	-6.67378000	2.01316200	0.68416700
F	-5.75054600	2.68536800	-1.16372800
F	-4.92032200	3.30802600	0.74452400

F	-4.08420100	-3.63451200	0.47881400
F	-5.04434900	-3.08478900	-1.39127300
F	-6.09004400	-2.78281400	0.48885500
S	0.02269100	-1.73547200	-1.28903600
C	3.65565500	0.54933800	1.65792300
H	2.81631500	1.19207400	1.94262000
H	4.55145500	1.03894600	2.06182400
H	-2.26054700	-2.03850700	-0.00330100
C	2.23230200	3.60201600	0.73341500
H	-0.76077400	1.29965500	0.47958500
H	1.36451100	4.25811100	0.73941700
H	1.28204300	1.16424000	0.40760800
C	5.10181400	-0.08758400	-0.36153500
C	5.16417100	-1.15064100	-1.27609800
C	6.32223200	0.42181400	0.11696900
C	6.38919000	-1.68693200	-1.68319100
H	4.25992500	-1.58693300	-1.68454400
C	7.54533300	-0.10921500	-0.28765600
H	6.32774100	1.24710200	0.82319800
C	7.58623200	-1.17143500	-1.19200900
H	6.39848600	-2.51304200	-2.38921600
H	8.46762800	0.30892900	0.10711600
H	8.53784900	-1.58937300	-1.50842500
C	3.47673500	-0.79550300	2.34465400
C	2.29957600	-1.13134800	2.88519900
H	1.42998000	-0.48225700	2.82450600
H	2.80513000	3.55293500	1.65579500
H	2.15910000	-2.07651200	3.40346000
C	1.84232100	3.08941900	-1.67001700
H	1.53872100	2.12078600	-2.08510800
H	0.94813500	3.70963600	-1.55063700
H	2.48305800	3.56549300	-2.42432900
C	4.67390700	-1.71028900	2.46024200
H	5.52932300	-1.18573100	2.90649800
H	4.44249800	-2.57881200	3.08454100
H	5.01081000	-2.07369700	1.48348800

AT-5-3

0 imaginary frequencies

H = -2074.534264

G = -2074.640235

E(M06-2X-DCM) = -2074.933297

C	3.48528700	0.15612500	0.03324500
C	3.45912300	1.56159500	-0.65286700

H	2.57111600	2.08804200	-0.28764300
H	4.31538500	2.14688800	-0.30032700
C	3.43546900	1.60909000	-2.17288600
C	2.41039900	-0.75581500	-0.63509100
H	2.25283500	-1.66124600	-0.04843500
H	2.74910000	-1.05412600	-1.63406900
N	1.10374900	-0.12599300	-0.77423400
C	-0.06598700	-0.59304600	-0.25087300
N	-1.13826700	0.19066100	-0.65105500
C	-2.51359400	0.05716400	-0.37539100
C	-3.16701000	-1.18094200	-0.30735200
C	-3.26215400	1.23395100	-0.25013100
C	-4.54410100	-1.21950300	-0.09456300
C	-4.64103200	1.17770700	-0.05387100
H	-2.76953100	2.20022100	-0.30985200
C	-5.29439100	-0.04982700	0.03281100
H	-6.36687700	-0.09479800	0.17738500
C	-5.41394400	2.45758700	0.12897800
C	-5.23172200	-2.55610200	0.03164300
F	-6.69790300	2.32900300	-0.26527300
F	-4.86911500	3.47494900	-0.57769300
F	-5.43321400	2.84702500	1.42363400
F	-6.51264600	-2.49774000	-0.39710000
F	-5.26439400	-2.97634700	1.31509600
F	-4.60598200	-3.51349800	-0.68489700
S	-0.18489500	-1.91459400	0.77350300
C	3.07002900	0.29149300	1.54846000
H	3.12313600	-0.71632400	1.97317500
H	2.01002600	0.57591700	1.56399800
H	-2.60727700	-2.09729900	-0.42531500
C	2.43291800	2.23103600	-2.81221800
H	-0.88945300	1.10449800	-1.01203000
H	2.40764900	2.31595200	-3.89564600
H	1.04492700	0.53687200	-1.54059300
C	4.86601200	-0.52521700	-0.05607700
C	4.99447800	-1.91213400	-0.24830200
C	6.05419600	0.20584900	0.11884000
C	6.24487900	-2.53314800	-0.28696800
H	4.11690700	-2.53684500	-0.37036900
C	7.30507100	-0.41011200	0.08106200
H	6.01551900	1.27331700	0.30162300
C	7.40953500	-1.78523800	-0.12692300
H	6.30110700	-3.60734500	-0.44257100
H	8.19999100	0.19124200	0.21892600

H	8.38332500	-2.26619200	-0.15899700
C	3.84477400	1.24107500	2.44677700
C	4.87278300	0.80810200	3.18626600
H	5.21062100	-0.22386300	3.15040000
H	1.62597000	2.72438200	-2.27186700
H	5.41320800	1.47217300	3.85695700
C	4.58749400	1.01013100	-2.94335900
H	4.46528100	1.16645900	-4.01949400
H	5.53776100	1.46374400	-2.63468900
H	4.69398200	-0.06435100	-2.75885600
C	3.35860300	2.66938600	2.55602600
H	3.94600200	3.23432300	3.28662400
H	3.40850400	3.20602700	1.60089700
H	2.30734700	2.69739100	2.87441900

AT-5-4

0 imaginary frequencies

H = -2074.531320

G = -2074.637757

E(M06-2X-DCM) = -2074.930032

C	3.57309400	0.20445500	-0.36011000
C	4.04188600	1.31856000	-1.36110800
H	4.61122700	2.05959200	-0.79065700
H	4.74373900	0.85234000	-2.06065800
C	2.99875100	2.04181600	-2.21023200
C	2.50701600	-0.71950400	-1.03567700
H	2.37579600	-1.64259700	-0.47689300
H	2.86282600	-1.00229700	-2.03481300
N	1.17548300	-0.13952500	-1.14049300
C	0.04336700	-0.64939900	-0.58659200
N	-1.02833400	0.21676500	-0.73816600
C	-2.38222100	0.06314400	-0.38078000
C	-3.06969700	-1.15507700	-0.47044000
C	-3.07988500	1.21590600	0.00128700
C	-4.42736800	-1.20175300	-0.15760800
C	-4.44109700	1.15450300	0.29472500
H	-2.56081000	2.16777700	0.06731100
C	-5.12673200	-0.05644900	0.22493200
H	-6.18612000	-0.10404600	0.44527200
C	-5.15514500	2.39928200	0.75230700
C	-5.14730200	-2.52636700	-0.20397200
F	-4.63051600	3.51187300	0.18817500
F	-5.06618000	2.56084300	2.09176100
F	-6.46840900	2.36647800	0.44374400

F	-4.61213200	-3.35832200	-1.12208800
F	-6.45533200	-2.37027900	-0.50886200
F	-5.09352300	-3.16073000	0.98765900
S	-0.04097800	-2.13426200	0.19590500
C	2.94362000	0.84182800	0.93163900
H	2.44916500	0.03634300	1.48878300
H	2.14708700	1.52008600	0.60962900
H	-2.55104600	-2.04883600	-0.78539400
C	2.27250700	3.08084700	-1.77020000
H	-0.78393000	1.17074400	-0.97854200
H	1.57652200	3.60101700	-2.42510200
H	1.12743500	0.77399600	-1.57804400
C	4.77146500	-0.69269200	0.03446000
C	4.55293400	-1.89625400	0.73119000
C	6.10427400	-0.33420600	-0.21931800
C	5.61127300	-2.70979500	1.13286800
H	3.54486200	-2.20699300	0.98902400
C	7.16811000	-1.14486300	0.18538100
H	6.33810600	0.59478500	-0.72568400
C	6.92885900	-2.34079600	0.85823200
H	5.40126400	-3.63351200	1.66550800
H	8.18687300	-0.83230600	-0.02876600
H	7.75517800	-2.97404100	1.16928300
C	3.87755900	1.59177800	1.87188400
C	4.06984700	2.91302100	1.76684900
H	3.58370000	3.51600100	1.00488800
H	2.37033000	3.47601700	-0.76394500
H	4.71897800	3.44910800	2.45480300
C	2.87679100	1.57831100	-3.64636700
H	3.83565200	1.70274200	-4.16699200
H	2.62554300	0.51227300	-3.71690900
H	2.11841900	2.14492400	-4.19564100
C	4.52424600	0.81055700	2.99262100
H	5.10262100	1.46799200	3.64930200
H	3.75965200	0.30966400	3.60206000
H	5.19043400	0.02686400	2.61897800

AT-6

0 imaginary frequencies

H = -2153.108644

G = -2153.222908

E(M06-2X-DCM) = -2153.547427

C	3.49690700	0.37287200	-0.48413900
C	3.33139700	-0.38783100	-1.85456700

H	2.34431500	-0.11112900	-2.24265600
H	4.06885300	0.03260500	-2.55207800
C	3.44512800	-1.90553500	-1.85729800
C	2.34857100	-0.03075900	0.47591800
H	2.52705900	0.38744300	1.47490200
H	2.30158500	-1.11473000	0.57655700
N	1.03709700	0.40995500	0.00878800
C	-0.13436000	-0.23288700	0.30005800
N	-1.21767500	0.48227200	-0.19496300
C	-2.59865700	0.24174600	-0.06838600
C	-3.18456300	-0.27579900	1.09535400
C	-3.42090200	0.62322600	-1.13603800
C	-4.56924000	-0.41925400	1.16208900
C	-4.80527800	0.48659500	-1.04698000
H	-2.98110400	1.03371100	-2.04047500
C	-5.39282800	-0.04184700	0.10043500
H	-6.46889800	-0.14072200	0.17394400
C	-5.66140000	0.85671000	-2.22976900
C	-5.18727800	-1.02646000	2.39667700
F	-6.90245000	1.22996500	-1.85373300
F	-5.80127000	-0.17944500	-3.08703100
F	-5.12354200	1.87858300	-2.93524300
F	-4.45277100	-0.77811000	3.50161800
F	-5.29851700	-2.36828900	2.28586100
F	-6.43110300	-0.54462300	2.61761200
S	-0.24489600	-1.69879600	1.09911100
C	3.40611800	1.90417000	-0.83459800
H	2.61419800	2.02489200	-1.58405800
H	4.33238200	2.18967900	-1.34766500
H	-2.56670400	-0.55587900	1.93610400
C	2.32317600	-2.64394800	-1.80056400
H	-0.98622500	1.12989000	-0.93950200
H	0.96385200	1.41700400	-0.09673200
C	4.85878400	0.02409100	0.14894100
C	4.97983900	-0.75350000	1.31176300
C	6.05110900	0.44138300	-0.46952900
C	6.23119800	-1.08634000	1.83851700
H	4.09877100	-1.12170000	1.82464300
C	7.30086000	0.11232300	0.05174700
H	6.01315500	1.02238100	-1.38644500
C	7.39916900	-0.65351300	1.21475300
H	6.28487400	-1.69014500	2.74063300
H	8.19966200	0.45293000	-0.45587100
H	8.37186900	-0.91140700	1.62440800

C	3.15102200	2.89358000	0.29260800
C	2.05820500	3.67890300	0.23972400
H	1.40473200	3.56512700	-0.63026900
H	1.37481200	-2.10962000	-1.73917000
C	4.83195200	-2.49358900	-1.99400100
H	4.80861400	-3.56524400	-2.20561700
H	5.37494500	-2.00625000	-2.81506100
H	5.43441400	-2.34514100	-1.09133100
C	4.19947300	2.98674900	1.37535900
H	4.00318500	3.79577700	2.08202700
H	4.28279100	2.05401600	1.94411500
H	5.18874800	3.15776100	0.93202000
C	1.61347400	4.74944000	1.19731400
H	2.26877200	4.85150000	2.06537300
H	1.56769900	5.72533800	0.69507700
H	0.60107600	4.54340300	1.56994900
C	2.17718800	-4.13898700	-1.79202900
H	1.56832300	-4.47581600	-2.64245000
H	3.13098700	-4.67139500	-1.82938800
H	1.64814900	-4.46110500	-0.88546800

AT-6-1

0 imaginary frequencies

H = -2153.107164

G = -2153.220733

E(M06-2X-DCM) = -2153.545669

C	3.34886900	-0.39305700	0.28019000
C	3.13909300	0.34416600	1.65980200
H	2.05868900	0.31255900	1.86439200
H	3.61180500	-0.27110400	2.43421300
C	3.64237500	1.76744800	1.82802500
C	2.21355500	-0.02868500	-0.71666000
H	2.41674700	-0.49053500	-1.69090000
H	2.14471200	1.04625400	-0.87361200
N	0.89892300	-0.47502400	-0.26690400
C	-0.26103500	0.23282500	-0.40068800
N	-1.34415800	-0.51437900	0.04396700
C	-2.71892400	-0.20940600	0.02730200
C	-3.49895300	-0.67420300	1.09306400
C	-3.34002700	0.46175100	-1.03499300
C	-4.87796200	-0.46894900	1.10167600
C	-4.71682300	0.67499500	-1.00155700
H	-2.75485900	0.81077800	-1.87345300
C	-5.49902100	0.21465000	0.05881000

H	-6.56910900	0.38191100	0.06877700
C	-5.36838500	1.45572100	-2.11535800
C	-5.70333900	-1.04344000	2.22282000
F	-5.40365000	2.77755700	-1.83913500
F	-6.64568000	1.06080800	-2.31706800
F	-4.70838800	1.31063000	-3.28388800
F	-6.82890800	-0.33123900	2.43503100
F	-5.01403500	-1.07776800	3.38573600
F	-6.08296200	-2.31520300	1.95632100
S	-0.36481300	1.80057400	-0.97963100
C	3.26671400	-1.92940600	0.62069100
H	2.45262100	-2.05910800	1.34473200
H	4.18395700	-2.19807400	1.15931000
H	-3.02892800	-1.18725700	1.92708300
C	4.58366300	2.01500100	2.75436700
H	-1.10460100	-1.26857400	0.67731300
H	0.80317700	-1.48512000	-0.23862300
C	4.72330600	-0.02947700	-0.31090800
C	4.87985000	0.65361400	-1.52692900
C	5.89349900	-0.35323600	0.39815600
C	6.14629000	0.97885800	-2.02231400
H	4.01516600	0.94468800	-2.11320800
C	7.15769800	-0.03223800	-0.09117100
H	5.82165500	-0.85701100	1.35772300
C	7.29245600	0.63415700	-1.31065700
H	6.22822900	1.50508800	-2.96978200
H	8.03948200	-0.30009400	0.48527300
H	8.27709800	0.88489900	-1.69561600
C	3.06191600	-2.92226700	-0.51299200
C	1.97190200	-3.71356600	-0.50353000
H	1.28287700	-3.60160600	0.33890300
H	4.96172600	1.16382500	3.32349500
C	3.01277300	2.83678100	0.96786900
H	3.38976900	2.79272900	-0.06265400
H	1.92464300	2.71488500	0.90978800
H	3.21636300	3.84394100	1.33949400
C	4.15737000	-3.01617200	-1.54833700
H	4.25232400	-2.09153400	-2.12817700
H	5.12842000	-3.16389900	-1.05884100
H	4.00478500	-3.83978000	-2.24897700
C	1.57511400	-4.79111000	-1.47443200
H	0.57632900	-4.59621300	-1.88765100
H	2.26520200	-4.88926300	-2.31556700
H	1.51869500	-5.76596500	-0.97125600

C	5. 21627800	3. 32671900	3. 12418300
H	6. 29407500	3. 30941400	2. 90985900
H	4. 79004700	4. 17956000	2. 59004900
H	5. 11566100	3. 51934200	4. 20103800

AT-6-2

0 imaginary frequencies

H = -2153.107068

G = -2153.220747

E(M06-2X-DCM) = -2153.545601

C	-3. 34820200	0. 38419700	0. 28804200
C	-3. 13504700	-0. 38510800	1. 64958600
H	-2. 05418500	-0. 35783400	1. 85235400
H	-3. 60615900	0. 21162900	2. 43931500
C	-3. 63746400	-1. 81214800	1. 78558600
C	-2. 21377700	0. 04502500	-0. 71874900
H	-2. 41946600	0. 52857200	-1. 68186000
H	-2. 14298000	-1. 02591200	-0. 90030800
N	-0. 89930800	0. 48384100	-0. 26117000
C	0. 26186600	-0. 21890500	-0. 41161500
N	1. 34393300	0. 52066000	0. 04728500
C	2. 72011200	0. 22314000	0. 02146100
C	3. 50250100	0. 69043000	1. 08448800
C	3. 34174900	-0. 43448000	-1. 04909400
C	4. 88365700	0. 50088300	1. 08285500
C	4. 72154600	-0. 62923000	-1. 02764500
H	2. 75543400	-0. 78196500	-1. 88733500
C	5. 50583400	-0. 16644000	0. 03005400
H	6. 57976700	-0. 30701400	0. 02379700
C	5. 37613800	-1. 38458600	-2. 15721000
C	5. 69444300	0. 96911600	2. 26287700
F	4. 70382600	-1. 23612100	-3. 31825500
F	5. 43571400	-2. 70902300	-1. 89800200
F	6. 64485700	-0. 96585200	-2. 36468300
F	6. 96633300	1. 25629200	1. 91554900
F	5. 75031300	0. 02937000	3. 23320900
F	5. 16322000	2. 08012500	2. 82389100
S	0. 36694900	-1. 77417200	-1. 02334200
C	-3. 26788700	1. 91216100	0. 66445200
H	-2. 45261300	2. 02620400	1. 38978900
H	-4. 18456600	2. 16651700	1. 21092000
H	3. 03463000	1. 20896400	1. 91641400
C	-4. 57579300	-2. 08177500	2. 70878000
H	1. 10322000	1. 26313900	0. 69389600

H	-0.80549000	1.49329100	-0.21155500
C	-4.72304600	0.03269400	-0.30937900
C	-4.88058900	-0.62126200	-1.54119100
C	-5.89254000	0.33746500	0.40918800
C	-6.14734400	-0.93653900	-2.04216900
H	-4.01643600	-0.89689100	-2.13565900
C	-7.15706100	0.02627600	-0.08563300
H	-5.81988700	0.81823100	1.38043500
C	-7.29284500	-0.61086500	-1.32054300
H	-6.23005800	-1.44004200	-3.00184100
H	-8.03828400	0.27880500	0.49853500
H	-8.27774200	-0.85389700	-1.70976700
C	-3.06693500	2.93182200	-0.44595100
C	-1.97816700	3.72449700	-0.41988900
H	-1.28738700	3.59390100	0.41841100
H	-4.95231400	-1.24433600	3.29891500
C	-3.01004100	-2.86053400	0.89856600
H	-1.92184400	-2.73830400	0.84229800
H	-3.21429200	-3.87637200	1.24535500
H	-3.38819500	-2.79044500	-0.13006700
C	-4.16456900	3.04857700	-1.47666200
H	-4.25922900	2.13800300	-2.07838000
H	-5.13487900	3.18296800	-0.98188700
H	-4.01471900	3.88901200	-2.15763800
C	-1.58506000	4.82528900	-1.36593300
H	-0.58638600	4.64238100	-1.78484800
H	-2.27646400	4.94136000	-2.20369800
H	-1.53026700	5.78831900	-0.84031200
C	-5.20673100	-3.40206400	3.04981300
H	-5.10180000	-3.62019000	4.12137900
H	-6.28536800	-3.37993600	2.84022500
H	-4.78245400	-4.24185800	2.49389800

AT-6-3

0 imaginary frequencies

H = -2153.107031

G = -2153.221216

E(M06-2X-DCM) = -2153.545836

C	-3.25985200	0.07241300	0.10116500
C	-3.24155300	1.01351700	-1.15079700
H	-2.37970000	0.72051200	-1.76013700
H	-4.11467500	0.79177700	-1.77291600
C	-3.16207000	2.51834300	-0.92466200
C	-2.14975800	0.52833000	1.09791200

H	-1.99428000	-0.22021700	1.87482300
H	-2.45326100	1.46430600	1.58190500
N	-0.84950800	0.74633200	0.47952900
C	0.30430300	0.08952400	0.77506400
N	1.39476100	0.67428800	0.14792000
C	2.74921800	0.28771800	0.12811100
C	3.70662900	1.30716600	0.05304400
C	3.16887800	-1.04929600	0.09550400
C	5.06220400	0.99905400	-0.04789700
C	4.52971500	-1.33968900	0.01058100
H	2.44142600	-1.84713100	0.13067100
C	5.48759500	-0.32768300	-0.06312800
H	6.54004000	-0.56867400	-0.14927400
C	4.97637100	-2.78025700	0.03031300
C	6.07369400	2.11473100	-0.07538500
F	6.12754600	-2.95266400	-0.65776100
F	4.05204800	-3.60118500	-0.51118400
F	5.20231000	-3.21114500	1.29061600
F	6.44840600	2.47856100	1.17175400
F	5.57889800	3.22288100	-0.67433500
F	7.19444100	1.75962100	-0.73775100
S	0.39704900	-1.24912900	1.78356600
C	-2.88469300	-1.38927300	-0.35524400
H	-2.76928800	-1.98823800	0.55585400
H	-1.88712100	-1.32983800	-0.80516600
H	3.39452400	2.34745000	0.06982200
C	-2.14013000	3.20567000	-1.47255500
H	1.24386400	1.61479400	-0.19806300
H	-0.80485500	1.56368800	-0.11989400
C	-4.62265500	0.06524600	0.82383100
C	-4.71880200	-0.04511900	2.22190200
C	-5.83071700	0.10575700	0.10435400
C	-5.95571500	-0.09488700	2.86936400
H	-3.82572500	-0.09837400	2.83421600
C	-7.06772900	0.05387100	0.74617300
H	-5.81619300	0.15847500	-0.97852100
C	-7.13922000	-0.04187000	2.13630100
H	-5.98636400	-0.17739500	3.95268800
H	-7.97832600	0.08694400	0.15338900
H	-8.10209400	-0.07883900	2.63835900
C	-3.82330600	-2.12072200	-1.30612600
C	-3.69094300	-1.97584400	-2.63582700
H	-2.89796700	-1.31510300	-2.98982100
H	-1.41643600	2.63400600	-2.06056800

C	-4.28985900	3.17147700	-0.16162800
H	-5.25232000	2.94597900	-0.63788100
H	-4.36623300	2.78809700	0.86181100
H	-4.18833500	4.25748100	-0.10888000
C	-4.79944300	-3.07078700	-0.65020900
H	-5.37377400	-2.57521100	0.13918100
H	-5.50791500	-3.51363900	-1.35432700
H	-4.25073600	-3.89367500	-0.17020300
C	-4.48142200	-2.62673800	-3.73685800
H	-5.29818800	-3.25362600	-3.37050700
H	-4.91513800	-1.87091400	-4.40608900
H	-3.83314800	-3.25701600	-4.36155100
C	-1.87473500	4.68655700	-1.45215800
H	-2.58197300	5.24516400	-0.83477400
H	-0.86587900	4.90093300	-1.07403900
H	-1.91837300	5.10213300	-2.46822600

AT-7

0 imaginary frequencies

H = -2231.670987

G = -2231.790814

E(M06-2X-DCM) = -2232.156489

C	-3.58038100	-0.10327300	-0.33514700
C	-3.53400000	1.33862900	0.28982300
H	-2.76997100	1.89699000	-0.25038400
H	-4.48406700	1.83177200	0.04399200
C	-3.30742600	1.45880400	1.79133500
C	-2.35904600	-0.92262000	0.13965900
H	-2.34976300	-1.91104400	-0.33679500
H	-2.42225900	-1.09395100	1.21745400
N	-1.09146200	-0.25300500	-0.12102900
C	0.10781800	-0.75498400	0.26772800
N	1.15343500	0.08158200	-0.10816200
C	2.54446100	-0.08883800	0.00511700
C	3.18251500	-1.33397300	-0.09141100
C	3.32370500	1.06722600	0.14801200
C	4.57328700	-1.40008400	-0.02720000
C	4.71372400	0.98319000	0.19995300
H	2.84424000	2.03929500	0.22020400
C	5.35306900	-0.25215200	0.11937500
H	6.43307200	-0.31957800	0.16660900
C	5.52094900	2.23551600	0.41956300
C	5.25522000	-2.73356500	-0.20435100
F	4.92760700	3.31655600	-0.13804500

F	6.75919700	2.13368000	-0.10731000
F	5.67134200	2.50778500	1.73562800
F	5.54486700	-2.96730900	-1.50653200
F	4.48718400	-3.75640600	0.21951300
F	6.42371600	-2.78892800	0.47237000
S	0.27021700	-2.18487500	1.12688800
C	-3.64249700	0.00873900	-1.91833300
H	-4.47862800	0.67251700	-2.15403600
H	-3.94593400	-0.98103900	-2.28026800
H	2.59815700	-2.23564300	-0.20380800
C	-2.21344000	2.04393900	2.32940300
H	0.87839900	1.03811600	-0.29857700
H	-1.10238000	0.45674300	-0.84652000
C	-4.87852500	-0.84920600	0.05566900
C	-4.88500100	-2.12388300	0.64349900
C	-6.12752900	-0.26965100	-0.23091500
C	-6.08185600	-2.78091200	0.94300600
H	-3.95701900	-2.62872400	0.88652700
C	-7.32327700	-0.92131200	0.06504500
H	-6.17756800	0.71290200	-0.69136400
C	-7.30774400	-2.18489800	0.65745900
H	-6.04638800	-3.76517100	1.40254500
H	-8.26856200	-0.43815000	-0.16839100
H	-8.23773400	-2.69583500	0.89096600
C	-2.40634500	0.41744800	-2.71889400
C	-2.13025900	1.69186700	-3.08859500
C	-4.44695000	0.93645200	2.64816300
H	-5.41077400	1.17468300	2.18462400
H	-4.42553500	-0.15510200	2.75479700
H	-4.45351200	1.36733700	3.65074200
C	-1.60373100	-0.77549600	-3.21319000
H	-0.59832300	-0.52772100	-3.55834700
H	-1.50525500	-1.54517700	-2.44151700
H	-2.13009100	-1.24695300	-4.05552900
C	-3.00470600	2.88620300	-2.76985100
H	-3.94101800	2.63453300	-2.27165300
H	-2.47492500	3.61021800	-2.13501100
H	-3.25093700	3.42019500	-3.69817500
C	-1.96383100	2.15021600	3.82037500
H	-0.94319100	1.81725100	4.05181300
H	-2.03120200	3.19498200	4.15748800
H	-2.64237400	1.55389800	4.43064900
C	-1.08600000	2.68970400	1.55139300
H	-1.26660200	2.78050200	0.47836800

H	-0.90313600	3.70290600	1.93560800
H	-0.14855800	2.13471600	1.69801300
C	-0.94826600	2.08727900	-3.95067600
H	-1.28589200	2.35434400	-4.96231800
H	-0.46150800	2.98463300	-3.54565300
H	-0.18689500	1.31293000	-4.05460900

AT-7-1

0 imaginary frequencies

H = -2231.670960

G = -2231.791877

E(M06-2X-DCM) = -2232.155531

C	3.45774100	0.01392700	0.53205200
C	3.33437200	1.03754700	1.72976700
H	2.62542900	0.60816800	2.44127500
H	4.29367000	1.04202100	2.26078400
C	2.95988000	2.48050700	1.41413600
C	2.27401400	0.17316200	-0.45166900
H	2.27532800	-0.64431100	-1.17344100
H	2.37203500	1.10867400	-1.01650500
N	0.97338600	0.15621400	0.21120400
C	-0.20036800	-0.03994900	-0.45920400
N	-1.28547400	0.08965800	0.39982400
C	-2.66596400	0.03916800	0.12863100
C	-3.23829700	0.56794000	-1.03700000
C	-3.49998800	-0.49853600	1.11666200
C	-4.62176200	0.53334600	-1.19941300
C	-4.88315300	-0.51512500	0.94274200
H	-3.07025500	-0.90840700	2.02616200
C	-5.45725500	-0.00567300	-0.21966100
H	-6.53128900	-0.02459700	-0.35914900
C	-5.75135000	-1.15806000	1.99232700
C	-5.23785000	1.16697000	-2.42150800
F	-5.22678900	-1.01253600	3.23114400
F	-5.88979300	-2.48608100	1.77951600
F	-6.99236200	-0.62834700	2.01037200
F	-4.40177700	1.14909700	-3.47816900
F	-5.56146000	2.46178100	-2.19227500
F	-6.37648600	0.53784000	-2.78696600
S	-0.30449900	-0.43005500	-2.08269300
C	3.42325300	-1.42098300	1.19483300
H	2.49500100	-1.47391100	1.76903500
H	4.23608700	-1.44687500	1.93380500
H	-2.60959100	0.99131100	-1.80695900

C	1.85417000	3.08439600	1.91075500
H	-1.06009400	-0.03929100	1.37956100
H	0.91015700	0.75909000	1.02265600
C	4.78849800	0.20993200	-0.22671900
C	4.86216200	0.31842400	-1.62445400
C	6.00294800	0.24619000	0.48141900
C	6.08720400	0.46967700	-2.28076000
H	3.96438200	0.28240900	-2.23083600
C	7.22696400	0.39662500	-0.16757200
H	6.00408400	0.14417800	1.56301200
C	7.27685700	0.51292900	-1.55767200
H	6.10279300	0.55236600	-3.36438000
H	8.14355900	0.42027100	0.41626600
H	8.22899500	0.63199400	-2.06730600
C	3.54985700	-2.64108500	0.29413600
C	2.50394700	-3.43753300	-0.02365600
C	3.97486900	3.21579700	0.56040200
H	3.84337600	4.29833300	0.57501400
H	4.98910400	3.00294200	0.91799100
H	3.95283500	2.88895000	-0.48605400
C	4.96104400	-2.96983500	-0.17334800
H	5.12872300	-4.04791300	-0.24494200
H	5.19900300	-2.53142800	-1.15028800
H	5.70093700	-2.57368400	0.52863300
C	1.08547800	-3.27907400	0.47642400
H	0.72540800	-4.23803200	0.87507100
H	0.96631400	-2.52769400	1.25807300
H	0.41138300	-3.01044200	-0.34770500
C	1.45784800	4.51341600	1.59732400
H	2.00607700	4.95722600	0.76616600
H	0.39027500	4.55967300	1.34368700
H	1.59292100	5.15960200	2.47678200
C	0.86151500	2.45459000	2.87083100
H	0.72670700	3.10767900	3.74378700
H	-0.13527700	2.36982400	2.41098000
H	1.14908200	1.47332900	3.25579200
C	2.63546800	-4.64057900	-0.93578600
H	3.57164600	-4.67233000	-1.49487100
H	2.54688200	-5.57775900	-0.36631500
H	1.81632200	-4.64604000	-1.66658300

AT-7-2

0 imaginary frequencies

H = -2231.671363

G = -2231.792413

E(M06-2X-DCM) = -2232.155546

C	3.08104300	0.00971600	0.18505600
C	2.72772100	-0.47880600	-1.27667400
H	2.67261900	-1.56851700	-1.22862800
H	1.70208300	-0.14119900	-1.47482300
C	3.60375400	-0.04788900	-2.44232200
C	1.96782400	-0.56221900	1.11327900
H	2.24782700	-0.41840300	2.16303500
H	1.83323700	-1.63087600	0.94407700
N	0.66277300	0.05298300	0.91242500
C	-0.48535700	-0.59375900	0.56568600
N	-1.55549900	0.28928400	0.51593300
C	-2.91762300	0.05077400	0.25051200
C	-3.59799300	-1.09369200	0.68925400
C	-3.63029000	1.05744800	-0.41294000
C	-4.96354700	-1.21896800	0.43921000
C	-4.99891100	0.92319000	-0.64068400
H	-3.11740900	1.95341000	-0.75074500
C	-5.67779300	-0.21951100	-0.22295000
H	-6.74267800	-0.32148700	-0.39234900
C	-5.72910500	1.99853100	-1.40160400
C	-5.67689800	-2.47737100	0.86644300
F	-5.66586700	1.79477300	-2.73682200
F	-5.20049100	3.22225400	-1.16741700
F	-7.03610400	2.04918200	-1.07004800
F	-6.97554500	-2.23775700	1.15706000
F	-5.11089900	-3.03038800	1.95987800
F	-5.65747000	-3.41263100	-0.10823800
S	-0.58292200	-2.22860200	0.20834400
C	3.04505100	1.58036900	0.24099000
H	2.23715700	1.89560600	-0.41811200
H	3.95904900	1.96763500	-0.22160600
H	-3.06746800	-1.86929300	1.22209400
C	4.55193200	-0.84556100	-2.98368100
H	-1.29734600	1.26719300	0.44580600
H	0.57767600	0.98067900	1.31154900
C	4.44759600	-0.57282700	0.59483300
C	4.56055800	-1.72584600	1.39060500
C	5.64508500	-0.00390400	0.12528600
C	5.80446000	-2.27296600	1.71528800
H	3.67603500	-2.22229400	1.77341200
C	6.88897300	-0.54677200	0.44556400
H	5.61681600	0.87237100	-0.51228900

C	6.97769200	-1.68586200	1.24697600
H	5.84844700	-3.16345800	2.33695100
H	7.79156200	-0.07506500	0.06518200
H	7.94614100	-2.10875200	1.49989300
C	2.89635700	2.24790800	1.60535600
C	1.88530300	3.10081400	1.90477400
C	3.29395100	1.32827400	-3.01684700
H	3.92019100	2.12311000	-2.58785100
H	3.42487800	1.36884200	-4.10138500
H	2.25344800	1.60506700	-2.81389100
C	4.03328300	1.95687200	2.56443600
H	4.99388300	2.15050900	2.07116900
H	4.00368800	2.55984000	3.47208700
H	4.06240000	0.90240800	2.86171100
C	0.79276800	3.53732800	0.94436200
H	0.84011000	4.62520800	0.79606800
H	0.83601400	3.07914800	-0.04518400
H	-0.20424200	3.34721000	1.37259200
C	5.42484100	-0.42762000	-4.14817300
H	5.29263800	0.61003800	-4.45805100
H	6.48467000	-0.56027000	-3.88987900
H	5.24146400	-1.06915800	-5.02216700
C	4.88466800	-2.24418100	-2.51475100
H	5.90046000	-2.27742600	-2.09835900
H	4.21189300	-2.63584100	-1.75170300
H	4.87142000	-2.93895000	-3.36621400
C	1.72848400	3.80435800	3.23888300
H	2.38935500	3.43501400	4.02290000
H	1.90615000	4.88405700	3.13114600
H	0.69807400	3.69952900	3.60482300

AT-7-3

0 imaginary frequencies

H = -2231.671040

G = -2231.791671

E(M06-2X-DCM) = -2232.155680

C	3.45705500	0.02008000	0.53283700
C	3.34408000	1.06930500	1.70915700
H	2.63514900	0.65937000	2.43214200
H	4.30524400	1.07895200	2.23670100
C	2.97735500	2.50758700	1.36433200
C	2.27081800	0.16574200	-0.44977500
H	2.26617400	-0.66555500	-1.15559000
H	2.37112800	1.08972400	-1.03291200

N	0.97233400	0.16726700	0.21750100
C	-0.20460500	-0.03154600	-0.44593800
N	-1.28670400	0.11864000	0.41387100
C	-2.66736900	0.06674400	0.14364600
C	-3.23829300	0.59033900	-1.02475500
C	-3.50282000	-0.45906800	1.13680600
C	-4.62226600	0.56123200	-1.18596200
C	-4.88638200	-0.46685100	0.96595000
H	-3.07416700	-0.86086900	2.05039400
C	-5.45930800	0.03733000	-0.19959900
H	-6.53456800	0.03928100	-0.32968500
C	-5.75815200	-1.08513100	2.02740100
C	-5.22496500	1.07815700	-2.46827700
F	-5.22692400	-0.93058300	3.26232300
F	-5.91412600	-2.41388000	1.83212800
F	-6.99233500	-0.53961500	2.04355300
F	-4.47370900	2.05482900	-3.01965200
F	-6.46360000	1.58157600	-2.26714500
F	-5.34297400	0.09806200	-3.39047300
S	-0.31640200	-0.44579400	-2.06295000
C	3.41698300	-1.40062700	1.22525300
H	2.48973000	-1.43720200	1.80242300
H	4.23128500	-1.41524100	1.96287800
H	-2.60940400	1.01882200	-1.79165100
C	1.87598800	3.12804400	1.84993100
H	-1.06032900	0.00184600	1.39490200
H	0.91549500	0.78018900	1.02179800
C	4.78605700	0.19249800	-0.23475100
C	4.85499500	0.27109100	-1.63473500
C	6.00335400	0.23681600	0.46800500
C	6.07838200	0.40139000	-2.29857800
H	3.95473000	0.22761700	-2.23693900
C	7.22572900	0.36645500	-0.18851700
H	6.00803000	0.15770700	1.55150200
C	7.27100200	0.45303700	-1.58094000
H	6.09032700	0.46112400	-3.38375100
H	8.14464900	0.39719200	0.39132200
H	8.22185700	0.55582200	-2.09647900
C	3.53578200	-2.63948000	0.34939700
C	2.48504800	-3.43587400	0.04786200
C	3.99505500	3.21900300	0.49378000
H	5.00871000	3.00760300	0.85387200
H	3.96901200	2.87075600	-0.54565400
H	3.86997500	4.30237000	0.48625000

C	4.94475700	-2.98631700	-0.11170400
H	5.10550400	-4.06665800	-0.16193700
H	5.18533800	-2.56888200	-1.09715100
H	5.68730500	-2.58112900	0.58229400
C	1.06783400	-3.25926900	0.54537500
H	0.39521800	-3.00012100	-0.28300700
H	0.70144500	-4.20885300	0.96033600
H	0.95415600	-2.49397300	1.31425900
C	1.48714200	4.55237300	1.50720300
H	1.62589600	5.21582700	2.37313100
H	2.03738300	4.97608200	0.66694100
H	0.41973200	4.59897600	1.25288700
C	0.88116000	2.52405800	2.82416000
H	1.16458800	1.55016400	3.23038100
H	0.75005800	3.19661300	3.68277800
H	-0.11632100	2.43379900	2.36689000
C	2.60926700	-4.65749900	-0.84032500
H	3.54339000	-4.70356100	-1.40187100
H	2.51964200	-5.58278100	-0.25186100
H	1.78755800	-4.67485800	-1.56802200

INT-12

0 imaginary frequency

H = -5236.813398

G = -5237.009413

E(M06-2X-DCM) = -5237.659624

E(M06-2X-cyclohexane) = -5237.635116

C	-0.78395300	4.96565500	0.35201100
C	-1.69814500	4.63640600	1.57925200
H	-1.62643200	3.56617800	1.80260200
H	-1.29521700	5.16814600	2.45177800
C	-3.15110400	5.01108200	1.44598300
C	-1.42772400	4.39747600	-0.93704100
H	-0.85801900	4.69606700	-1.82449800
H	-2.42646300	4.81984200	-1.05605600
N	-1.57991500	2.95085900	-0.88654400
C	-2.60269000	2.26433500	-1.45424600
N	-2.48456300	0.90028400	-1.24763200
C	-3.41377800	-0.12871500	-1.43275500
C	-4.80621900	0.06170300	-1.44272100
C	-2.91253800	-1.43649500	-1.53306100
C	-5.65582600	-1.03473900	-1.56883200
C	-3.78108800	-2.52028200	-1.65219900
H	-1.84075100	-1.60511000	-1.50537600

C	-5.16178200	-2.33454900	-1.68232900
H	-5.83389600	-3.17700300	-1.78952500
C	-3.22202500	-3.91316000	-1.65460900
C	-7.14402900	-0.82480200	-1.47316200
F	-4.04308100	-4.80051200	-2.25013400
F	-3.01456900	-4.36744700	-0.38483500
F	-2.02314100	-3.98446500	-2.28175800
F	-7.52226100	0.39266600	-1.90462000
F	-7.57233000	-0.93713700	-0.18613200
F	-7.82948500	-1.74586200	-2.18637300
S	-3.83517300	2.99919800	-2.34153700
H	-5.21226900	1.05883400	-1.35630500
C	-4.16218900	4.14210100	1.48284100
H	-1.57012100	0.59083100	-0.91807300
H	-0.79496100	2.41551100	-0.52306200
H	1.93743100	1.31994700	1.66433000
O	0.11050100	-1.46734400	0.95801500
O	2.30092100	-1.27040500	-0.39402000
P	1.15450400	-0.41024000	0.33814900
O	0.39011300	0.60318900	-0.42860700
C	1.38983500	-4.03775800	3.99689400
C	1.72117000	-4.30354500	2.67313900
C	1.19317500	-3.52273600	1.63210300
C	0.07124100	-2.10700700	3.28616600
C	0.53297600	-2.97439000	4.28810100
C	1.97220900	-2.19482100	-1.41153700
C	1.55356900	-3.47400300	-1.05380500
C	1.14561000	-4.34830700	-2.07678500
C	1.22925100	-3.97626800	-3.41371600
C	1.72391400	-2.71475500	-3.74200500
C	2.09651700	-1.79040700	-2.75400900
H	0.23554900	-2.78271800	5.31476700
H	1.81262100	-2.41836200	-4.78294100
C	1.49735100	-4.19284300	0.29451200
C	2.84560800	-4.90093600	0.65145000
H	3.07905200	-5.72339300	-0.03184700
H	3.65740600	-4.16710900	0.59191700
H	-0.30345700	-5.96664000	-1.98817900
H	1.35129500	-6.45249500	-1.61403200
C	0.46569400	-2.38775100	1.96481700
H	1.78833300	-4.65018900	4.80157500
H	0.91031800	-4.65820900	-4.19743200
C	2.65932700	-5.35487500	2.11846700
H	2.22163200	-6.36076200	2.17638600

H	3.60595200	-5.39028800	2.66878300
C	0.61940100	-5.64094000	-1.49864400
C	0.40486500	-5.27513100	-0.01759600
H	0.46956200	-6.13353000	0.65696100
H	-0.58663000	-4.82901400	0.10425900
C	2.63773600	-0.45300500	-3.16120300
C	4.03714300	-0.23915200	-3.14053900
C	1.76603900	0.55622100	-3.63358200
C	4.97159100	-1.25197700	-2.75206900
C	4.56893500	1.03963700	-3.55344500
C	2.31194800	1.82989800	-4.04817500
C	6.32175800	-1.01497800	-2.74997200
H	4.59627200	-2.22669500	-2.46031200
C	5.98315100	1.24940100	-3.52577500
C	3.69253000	2.03919000	-3.98701500
C	6.83863800	0.25479600	-3.13467500
H	7.00801800	-1.80420700	-2.45475100
H	6.36504200	2.21998400	-3.83378600
H	4.09773500	2.99835900	-4.30415700
H	7.91166600	0.42522400	-3.12410200
C	-0.82855300	-0.95617100	3.61413800
C	-2.17553000	-0.97786000	3.17060900
C	-0.34969900	0.13147100	4.38559700
C	-2.73580600	-2.06918300	2.43270900
C	-3.04668900	0.13411300	3.47763300
C	-1.23644000	1.23300900	4.69171600
C	-4.03825500	-2.05070800	2.00694400
H	-2.11596200	-2.92975200	2.20843300
C	-4.39783500	0.11714900	3.00746100
C	-2.55351400	1.20742500	4.22543000
C	-4.88325400	-0.93912800	2.28444300
H	-4.42518800	-2.89115300	1.43964800
H	-5.03229300	0.96949400	3.23890800
H	-3.21231400	2.04376900	4.45014500
H	-5.90168800	-0.93235800	1.90787700
C	-0.46702200	1.37773500	-4.19514400
H	-1.54040400	1.22425900	-4.25189500
C	0.34788200	0.37940800	-3.72938000
H	-0.08184100	-0.56956000	-3.42835800
C	0.07571200	2.63374800	-4.59224700
H	-0.59086300	3.41273100	-4.95070700
C	1.42565400	2.84933000	-4.52006500
H	1.85397400	3.80010000	-4.82934700
C	1.43001900	1.28691900	5.60260700

H	2.46044500	1.32083200	5.94390000
C	0.54969900	2.36386500	5.90787700
H	0.90962900	3.20444800	6.49504100
C	-0.74450100	2.33368500	5.46198200
H	-1.42938100	3.14775900	5.68788500
C	0.99588900	0.21191500	4.87095000
H	1.68258000	-0.59659000	4.64929200
N	2.11661600	0.32142800	1.52744600
S	3.57547300	-0.14421100	2.24160600
C	4.87143400	-0.05728500	0.85646800
O	3.51388900	-1.54210700	2.63775100
O	3.91372600	0.93173600	3.16449600
F	6.00166100	0.38457200	1.40664300
F	5.06730100	-1.26940100	0.35320900
F	4.48216100	0.78599300	-0.09658100
C	0.64142000	4.41724700	0.58032900
C	1.16541900	4.23199500	1.87214100
C	1.49616700	4.13661900	-0.50196200
C	2.48376200	3.81414200	2.07465700
H	0.55070500	4.40951200	2.74680400
C	2.81317400	3.71818800	-0.30645600
H	1.13754400	4.23592500	-1.52063300
C	3.31966600	3.56503400	0.98425800
H	2.85350800	3.67765700	3.08677900
H	3.43634600	3.49945800	-1.16903900
H	4.34383500	3.24136000	1.14271000
C	-0.71252900	6.52798500	0.20468500
H	-1.73274000	6.90931800	0.08028300
H	-0.33816900	6.92243200	1.16054100
C	0.14215700	7.06849400	-0.91067700
C	-0.31888500	7.77976900	-1.94151000
H	-1.37745800	8.00554300	-2.05566600
H	-3.99299000	3.07205000	1.58240200
H	-3.37891500	6.07223300	1.34238900
H	1.21127700	6.87257300	-0.83973200
H	-5.19608700	4.46530000	1.39905600
H	0.34415700	8.16813200	-2.71030300

INT-12'

0 imaginary frequency

H = -5236.796689

G = -5236.995619

E(M06-2X-DCM) = -5237.655289

E(M06-2X-cyclohexane) = -5237.625075

O	-0.83445400	-2.31161100	0.64075200
O	-2.76999500	-0.63733200	0.22866200
P	-1.14203900	-0.71666200	0.39876300
O	-0.53056700	-0.20899200	-0.87225900
C	-1.80323300	-4.89432500	-2.51166200
C	-2.76822200	-4.50406200	-1.58869100
C	-2.41989000	-3.70521000	-0.48997200
C	-0.11085800	-3.62632700	-1.27288600
C	-0.48431400	-4.48240200	-2.32478100
C	-3.59926300	-1.07350900	1.26823000
C	-3.85316700	-2.43801600	1.41446700
C	-4.54590400	-2.88795500	2.54995900
C	-5.07460500	-1.98504300	3.46498700
C	-4.91947000	-0.61999400	3.23081200
C	-4.17762800	-0.13157200	2.14201600
H	0.28586600	-4.81186400	-3.01578100
H	-5.36383300	0.09987800	3.91166700
C	-3.59126100	-3.61544700	0.47914400
C	-4.78648600	-3.83093600	-0.51030500
H	-5.02440200	-2.87302600	-0.98817800
H	-5.69081900	-4.18240100	-0.00402200
H	-5.59246600	-4.77541000	2.32951300
H	-4.34950300	-4.80278500	3.57568500
C	-1.12066700	-3.21285400	-0.38281000
H	-2.06356700	-5.52405200	-3.35890300
H	-5.61354100	-2.33224800	4.34294600
C	-4.24791000	-4.82239400	-1.56521900
H	-4.72248200	-4.69753900	-2.54554200
H	-4.42570600	-5.86379500	-1.26219900
C	-4.59161600	-4.39987000	2.58558800
C	-3.55220100	-4.79009300	1.51407200
H	-2.55349700	-4.82727300	1.96393200
H	-3.74640300	-5.76238000	1.05039000
C	-4.11150600	1.34989400	1.93932300
C	-3.45426300	2.16950100	2.88840500
C	-4.82871700	1.93738200	0.86701600
C	-2.68643400	1.63494600	3.97207400
C	-3.53555200	3.60800900	2.76927300
C	-4.88465300	3.37713600	0.75007000
C	-2.06564800	2.45471500	4.87672400
H	-2.56442200	0.56226000	4.04640200
C	-2.88348000	4.42755100	3.74345500
C	-4.24613800	4.17051100	1.70664200
C	-2.17240000	3.87053000	4.77107800

H	-1.46381700	2.01974900	5.66920200
H	-2.96239500	5.50766400	3.64234100
H	-4.30241100	5.25384500	1.61994600
H	-1.67406800	4.50337300	5.50057000
C	1.33030700	-3.25278200	-1.12922500
C	1.98062300	-2.54932900	-2.17370000
C	2.07445000	-3.70789800	-0.01118900
C	1.27747400	-1.99969600	-3.29563300
C	3.41228100	-2.35500300	-2.12311400
C	3.49548300	-3.45060200	0.05297100
C	1.94150100	-1.36505200	-4.31415100
H	0.19678300	-2.07336000	-3.32442700
C	4.07016700	-1.70988700	-3.21938600
C	4.12859000	-2.79847500	-1.00843900
C	3.35963200	-1.23257000	-4.28905600
H	1.37583800	-0.95757200	-5.14726200
H	5.15246900	-1.60970100	-3.17992700
H	5.20152700	-2.62551500	-0.96316100
H	3.87288600	-0.75133100	-5.11789800
C	-6.22932500	1.76889300	-1.13325100
H	-6.76312100	1.15768300	-1.85639500
C	-5.54356400	1.16892100	-0.10830500
H	-5.54746000	0.08820500	-0.02251100
C	-6.25991500	3.18726900	-1.25606800
H	-6.80672200	3.64665200	-2.07501000
C	-5.60882900	3.96327000	-0.33499100
H	-5.63313700	5.04819600	-0.40808500
C	2.23752100	-4.86131900	2.13778800
H	1.76314900	-5.41428000	2.94401900
C	3.63049100	-4.57777200	2.20878700
H	4.20524800	-4.90982300	3.06905200
C	4.23864900	-3.89718800	1.18985600
H	5.30447700	-3.68398400	1.22220000
C	1.49060500	-4.44785300	1.06624200
H	0.43406900	-4.68417000	1.02980000
C	-1.40879200	2.55655800	-3.32822600
C	-2.03342000	2.81507000	-1.92348200
H	-3.12424100	2.82883100	-2.03811100
H	-1.79722000	1.98050800	-1.25841500
C	-1.59897100	4.10095400	-1.26710900
C	0.13286700	2.69529000	-3.23865000
H	0.34771100	3.72682400	-2.94360400
H	0.57567200	2.51205500	-4.22548600
N	0.76606200	1.80387600	-2.25580800

C	1. 98758100	1. 96417300	-1. 77305300
N	2. 44439100	1. 22789300	-0. 75778000
C	3. 75831000	1. 34750600	-0. 19191200
C	3. 90224500	1. 88307200	1. 09181100
C	4. 86330900	0. 87951000	-0. 89909200
C	5. 17702700	1. 96016700	1. 65174700
C	6. 13321100	0. 96724500	-0. 32477100
H	4. 72492500	0. 43843600	-1. 87960900
C	6. 29609100	1. 50815000	0. 94815500
H	7. 28225600	1. 57688900	1. 39065100
C	7. 31289100	0. 46645100	-1. 11489900
C	5. 34399500	2. 49106000	3. 05478300
F	8. 45596600	0. 49401000	-0. 40430100
F	7. 50835600	1. 20131100	-2. 23235400
F	7. 12358600	-0. 81437000	-1. 52766900
F	6. 57112800	3. 03400500	3. 23150700
F	5. 20816100	1. 51298800	3. 97324100
F	4. 43234300	3. 44129200	3. 33804100
S	3. 12525900	3. 17891200	-2. 40377700
H	3. 02893700	2. 21110900	1. 64616100
H	1. 81266200	0. 59284900	-0. 24292800
H	0. 20522700	1. 03467100	-1. 83535900
C	-0. 93058300	4. 17609200	-0. 11335500
H	-0. 64775100	3. 29286300	0. 45591300
H	2. 37925900	3. 52914200	-3. 46550200
H	-0. 67131400	5. 13442000	0. 32972300
N	-0. 82388300	0. 00601800	1. 80589800
S	0. 65236700	0. 23813400	2. 32704400
O	0. 86738200	1. 60388800	2. 82758700
O	1. 70520600	-0. 30808000	1. 42563200
C	0. 74611400	-0. 85278800	3. 84038100
F	-0. 17153200	-0. 47579200	4. 74315100
F	1. 95908800	-0. 74447600	4. 39213800
F	0. 52778300	-2. 12779400	3. 51020900
C	-1. 80052500	1. 18230500	-3. 91167200
C	-2. 67341500	0. 30326000	-3. 25745900
C	-1. 30001100	0. 78857300	-5. 16629900
C	-3. 02274500	-0. 92296300	-3. 82979300
H	-3. 08348200	0. 55162300	-2. 28718200
C	-1. 64981900	-0. 43169900	-5. 74211300
H	-0. 62952900	1. 44320300	-5. 71809000
C	-2. 51482500	-1. 29875600	-5. 07118200
H	-3. 68835900	-1. 58857400	-3. 28770900
H	-1. 24877300	-0. 70212400	-6. 71567000

H	-2.78682300	-2.25373800	-5.51235300
C	-1.85793700	3.67930100	-4.32836000
H	-1.50231100	4.65257500	-3.96959200
H	-1.35500600	3.50330600	-5.29005300
C	-3.34204300	3.74995800	-4.56464500
C	-4.08103600	4.84977500	-4.41310100
H	-3.64921500	5.79301200	-4.08343800
H	-5.14812600	4.85256200	-4.61809100
H	-3.81804800	2.82809900	-4.89650900
H	-1.88793100	5.02747300	-1.76472500

INT-12' -1

0 imaginary frequency

H = -5236.801616

G = -5236.999510

E(M06-2X-DCM) = -5237.652666

E(M06-2X-cyclohexane) = -5237.625220

O	-0.74340600	-2.58710900	-0.89192100
O	-2.68528700	-1.01370300	-0.19677300
P	-1.05684100	-1.15527900	-0.15653500
O	-0.50868300	-0.00126600	-0.94822800
C	-1.81512100	-2.86043900	-4.93038000
C	-2.74690400	-3.10875500	-3.92771700
C	-2.36262700	-3.09311800	-2.57876700
C	-0.08759800	-2.48930100	-3.23259300
C	-0.49425800	-2.58641500	-4.57525800
C	-3.48646700	-1.98217400	0.41361100
C	-3.74074000	-3.18069200	-0.25406700
C	-4.40702200	-4.21184100	0.42753600
C	-4.90875200	-4.01070000	1.70861500
C	-4.75133700	-2.76168400	2.30812100
C	-4.03388400	-1.72670900	1.68621100
H	0.24804900	-2.41811000	-5.34995600
H	-5.17233300	-2.57609200	3.29190300
C	-3.50618200	-3.59704500	-1.70538800
C	-4.72860600	-3.21187200	-2.60683600
H	-4.96992300	-2.15593700	-2.43850200
H	-5.62163200	-3.80005700	-2.37385400
H	-5.46523900	-5.63514500	-0.82136300
H	-4.19204400	-6.36471100	0.15111700
C	-1.06258400	-2.72209200	-2.24222100
H	-2.10446200	-2.88397400	-5.97809700
H	-5.42732300	-4.80822800	2.23476300
C	-4.22540400	-3.40540800	-4.05424100

H	-4. 72756200	-2. 74299400	-4. 76862700
H	-4. 39695000	-4. 43320700	-4. 40392700
C	-4. 45699100	-5. 46605900	-0. 41758800
C	-3. 44564500	-5. 15289000	-1. 54062100
H	-2. 43618800	-5. 43230700	-1. 21793900
H	-3. 65563600	-5. 68039100	-2. 47638100
C	-3. 94147400	-0. 39956000	2. 37444400
C	-3. 20541300	-0. 26969200	3. 57668300
C	-4. 69334300	0. 69522400	1. 87844400
C	-2. 41539200	-1. 33359900	4. 11847100
C	-3. 22658800	0. 98439400	4. 29649800
C	-4. 69461500	1. 94718400	2. 60204400
C	-1. 71838000	-1. 17801500	5. 28679800
H	-2. 33947500	-2. 26146400	3. 56666600
C	-2. 49267100	1. 10094500	5. 51856900
C	-3. 96413300	2. 05677200	3. 78869300
C	-1. 76298800	0. 05069200	6. 00457300
H	-1. 10225300	-1. 99242400	5. 65589700
H	-2. 52631100	2. 04911800	6. 05046200
H	-3. 97922700	2. 99729400	4. 33646100
H	-1. 20308500	0. 15292800	6. 93026400
C	1. 34376700	-2. 17746500	-2. 92636700
C	1. 90188800	-0. 94377000	-3. 34634400
C	2. 16558100	-3. 15007900	-2. 30353400
C	1. 12276000	0. 10306500	-3. 93973800
C	3. 31572400	-0. 69948700	-3. 16790800
C	3. 56701000	-2. 86973000	-2. 08706200
C	1. 69835800	1. 27115700	-4. 36968700
H	0. 05310100	-0. 03408700	-4. 03697000
C	3. 88201900	0. 52516600	-3. 64841600
C	4. 10629500	-1. 65985100	-2. 53179900
C	3. 10105300	1. 48399800	-4. 23774800
H	1. 07823000	2. 04199100	-4. 82040800
H	4. 95373300	0. 67182400	-3. 53490400
H	5. 16387300	-1. 45751800	-2. 37587900
H	3. 54529800	2. 40524100	-4. 60591400
C	-6. 23094100	1. 68645500	0. 25180800
H	-6. 83520000	1. 59213300	-0. 64645800
C	-5. 49804700	0. 61605700	0. 69582400
H	-5. 53182500	-0. 31914700	0. 14864000
C	-6. 21606000	2. 92191700	0. 96092200
H	-6. 81275900	3. 75689000	0. 60249300
C	-5. 46807000	3. 04286000	2. 10273400
H	-5. 46386800	3. 97293200	2. 66733100

C	2. 49782600	-5. 34637000	-1. 28451100
H	2. 09733300	-6. 30903500	-0. 97838100
C	3. 87039200	-5. 05256900	-1. 04851800
H	4. 50290600	-5. 78856200	-0. 55978000
C	4. 38664500	-3. 84927200	-1. 44479600
H	5. 43564100	-3. 61378200	-1. 28192100
C	1. 67874700	-4. 43177600	-1. 89244900
H	0. 63897000	-4. 67992700	-2. 06964000
C	-1. 75749800	3. 93163600	-0. 89690800
C	-1. 76352700	4. 07157700	0. 65691400
H	-2. 80832100	4. 16678900	0. 97891400
H	-1. 40117500	3. 14019100	1. 10594500
C	-0. 98975400	5. 24180200	1. 20199500
C	-0. 31607600	3. 65789500	-1. 40208300
H	0. 29876100	4. 55094900	-1. 30865100
H	-0. 35277900	3. 38758400	-2. 46360400
N	0. 37034400	2. 55608800	-0. 71194500
C	1. 60945400	2. 55458400	-0. 24527500
N	2. 21606700	1. 40474400	0. 06363300
C	3. 55400000	1. 28533600	0. 57071800
C	4. 62401500	1. 48940300	-0. 29560800
C	3. 76688200	0. 90263900	1. 89729900
C	5. 92967400	1. 32363300	0. 17216000
C	5. 07656400	0. 75010000	2. 35104800
H	2. 92355400	0. 70976400	2. 55230900
C	6. 16162400	0. 95828200	1. 49522500
H	7. 17435400	0. 83596600	1. 85916800
C	5. 32207900	0. 30058200	3. 77096000
C	7. 06385700	1. 50803700	-0. 79973200
F	6. 53485900	0. 70761500	4. 21335600
F	5. 29253900	-1. 04333900	3. 87688700
F	4. 39420400	0. 79278600	4. 61465200
F	7. 02600200	0. 56935900	-1. 78256600
F	8. 26945400	1. 41773500	-0. 20782800
F	6. 99660300	2. 70803800	-1. 41769600
S	2. 55017600	4. 04819900	0. 01892000
H	4. 43528000	1. 74746700	-1. 33227100
H	1. 71365500	0. 51231900	-0. 05113100
H	-0. 05942700	1. 60987600	-0. 80793900
C	-0. 11632200	5. 18022200	2. 21410400
H	0. 11225900	4. 24320500	2. 71884300
H	1. 48037500	4. 75916700	0. 46073300
H	0. 37124000	6. 07156500	2. 60183800
N	-0. 66761000	-1. 35451900	1. 39291200

S	0.83375500	-1.47553600	1.89273200
O	1.06534000	-0.72945800	3.13750900
O	1.84212900	-1.30502500	0.81362700
C	0.97656900	-3.27074500	2.39057400
F	0.09995800	-3.54833400	3.36784700
F	2.21164700	-3.51081000	2.84227200
F	0.72841700	-4.07026200	1.35043900
C	-2.30791100	5.21959800	-1.54656000
C	-1.61874100	5.95507600	-2.52268000
C	-3.58129500	5.68527000	-1.16937700
C	-2.16867700	7.10921300	-3.08892700
H	-0.64184100	5.63780000	-2.87098600
C	-4.13175700	6.83582100	-1.73016800
H	-4.16008600	5.13902900	-0.43003500
C	-3.42598200	7.55850100	-2.69419500
H	-1.60564200	7.65263100	-3.84323600
H	-5.11717200	7.16698300	-1.41288100
H	-3.85363300	8.45587900	-3.13264400
C	-2.68816100	2.73021900	-1.27793300
H	-2.31152800	1.81049900	-0.81938200
H	-3.66825100	2.91504600	-0.82032600
C	-2.87239800	2.51957900	-2.75821300
C	-2.58267500	1.38819800	-3.40555400
H	-2.16462700	0.52880100	-2.88886300
H	-2.76831600	1.28427500	-4.47223400
H	-3.29610400	3.35696900	-3.31304100
H	-1.20284100	6.21025200	0.74884400

INT-12' -2

0 imaginary frequency

H = -5236.783695

G = -5236.978241

E(M06-2X-DCM) = -5237.637328

E(M06-2X-cyclohexane) = -5237.609816

O	0.16077100	2.49998900	-0.28475000
O	2.54819100	1.53381900	-0.67901000
P	1.00019600	1.09640900	-0.36608800
O	0.57759300	0.20908100	-1.49838900
C	0.22141900	5.05293700	-3.61102300
C	1.23783100	5.09001200	-2.66286400
C	1.18100000	4.27608500	-1.52212300
C	-0.93460200	3.34093000	-2.29373000
C	-0.86346500	4.20374400	-3.40195600
C	3.26161300	2.29439100	0.24968400

C	3. 00057100	3. 65864800	0. 37607900
C	3. 55085600	4. 36538200	1. 45687500
C	4. 46698700	3. 75730500	2. 30781800
C	4. 85024500	2. 44101700	2. 05397100
C	4. 25668200	1. 67678900	1. 03392200
H	-1. 68425500	4. 19052800	-4. 11301000
H	5. 61719500	1. 97485300	2. 66516000
C	2. 30426700	4. 64040700	-0. 56148000
C	3. 34619100	5. 24109800	-1. 56945800
H	3. 91583000	4. 41741500	-2. 01538900
H	4. 05945400	5. 91265300	-1. 08211000
H	3. 78827400	6. 50861200	1. 20909700
H	2. 67124500	6. 06813000	2. 49570700
C	0. 13657200	3. 36417100	-1. 38045000
H	0. 26007100	5. 68393500	-4. 49543300
H	4. 90379700	4. 30329100	3. 14020900
C	2. 49605900	5. 92865100	-2. 65719100
H	2. 99412500	5. 95098200	-3. 63331600
H	2. 27476700	6. 97239500	-2. 39245600
C	3. 01576400	5. 78137100	1. 49544600
C	1. 86731400	5. 73845400	0. 46228500
H	0. 94139600	5. 41330700	0. 95026000
H	1. 67529900	6. 70422700	-0. 01586400
C	4. 78178900	0. 30008600	0. 77331900
C	4. 72084200	-0. 69008500	1. 78496000
C	5. 48157600	0. 03579000	-0. 43344300
C	4. 01563800	-0. 49279400	3. 01555200
C	5. 39170500	-1. 95661700	1. 59387500
C	6. 11629500	-1. 24912300	-0. 62403900
C	4. 01797200	-1. 44593200	4. 00099900
H	3. 45996700	0. 42409800	3. 15555500
C	5. 37059200	-2. 92462400	2. 64800900
C	6. 05830200	-2. 20646000	0. 39216800
C	4. 71535200	-2. 67579900	3. 82401400
H	3. 47232400	-1. 26476000	4. 92312800
H	5. 89524500	-3. 86450600	2. 49225200
H	6. 55402300	-3. 16401600	0. 24734900
H	4. 71216200	-3. 41687300	4. 61875500
C	-2. 17203800	2. 51624600	-2. 12587200
C	-2. 47077600	1. 49360000	-3. 05811800
C	-3. 10838200	2. 85712700	-1. 11896600
C	-1. 54576700	1. 07258800	-4. 06874300
C	-3. 74717100	0. 81804400	-2. 99478800
C	-4. 37558300	2. 16455700	-1. 06125900

C	-1.86712100	0.08167500	-4.96054600
H	-0.56682000	1.53589700	-4.10521800
C	-4.04381200	-0.20964800	-3.94496900
C	-4.66396700	1.17212400	-2.00201500
C	-3.13547100	-0.56632600	-4.90550600
H	-1.14388500	-0.22183300	-5.71293400
H	-5.00332400	-0.71520300	-3.86987900
H	-5.61855500	0.65295400	-1.95497800
H	-3.37118400	-1.34997500	-5.62070300
C	6.32611100	0.71899800	-2.62608600
H	6.42337700	1.47692700	-3.39880300
C	5.63403000	1.00397000	-1.47824500
H	5.19824000	1.98732500	-1.35026500
C	6.92645200	-0.55748500	-2.81736800
H	7.47259700	-0.76523600	-3.73374200
C	6.82440600	-1.50931100	-1.83938200
H	7.28546600	-2.48601300	-1.96325700
C	-3.80380300	4.19599200	0.80391800
H	-3.59420800	4.97930000	1.52738200
C	-5.04180000	3.49663600	0.86843100
H	-5.76263300	3.74050200	1.64353400
C	-5.31865400	2.51772700	-0.04658500
H	-6.26367700	1.98320800	-0.01268100
C	-2.87565700	3.89129300	-0.15657300
H	-1.94176600	4.43991200	-0.19186400
C	1.57613600	-4.37630400	-0.29344900
C	0.51677600	-5.45706400	-0.71662300
H	0.44122100	-5.43628000	-1.81022300
H	0.95130200	-6.43623800	-0.46989200
C	-0.88385300	-5.43006000	-0.15386500
C	1.02672500	-2.93242300	-0.46212500
H	0.70215000	-2.77533700	-1.48856000
H	1.81347400	-2.20558100	-0.24336500
N	-0.10098800	-2.60907200	0.41141000
C	-1.31843700	-2.22644000	0.06419100
N	-2.21546800	-2.06471700	1.06255400
C	-3.59229000	-1.74775200	0.96750800
C	-4.42405700	-2.39284400	0.04882500
C	-4.12684900	-0.82849200	1.87760900
C	-5.78305700	-2.08032700	0.01638200
C	-5.49454000	-0.56574100	1.86179800
H	-3.47020300	-0.29454100	2.55441300
C	-6.33062700	-1.18094800	0.92916100
H	-7.39175700	-0.96046700	0.91282700

C	-6.09773600	0.36233300	2.88605200
C	-6.66048300	-2.67573200	-1.05223400
F	-6.63747500	-0.33347200	3.91417900
F	-7.09932400	1.10382300	2.35328200
F	-5.19274300	1.20898600	3.40649900
F	-6.76238500	-1.84468600	-2.12239000
F	-7.91631800	-2.89141600	-0.60939600
F	-6.17820900	-3.84945400	-1.51073700
S	-1.73967500	-1.86859100	-1.61593600
H	-4.02763000	-3.14303200	-0.62348600
H	-1.78585700	-1.90665000	1.97970900
H	0.10146900	-2.62321500	1.41254500
C	-1.98349300	-5.55192100	-0.90219900
H	-1.93555100	-5.61383400	-1.98740600
H	-0.71426700	-0.92870300	-1.69456400
H	-2.97328800	-5.61240400	-0.45623200
N	1.00455300	0.49985600	1.14233100
S	-0.18157100	0.42929600	2.17384800
O	-0.22408700	-0.90457700	2.84426300
O	-1.48686100	0.94769900	1.72917100
C	0.34420200	1.58597000	3.54501700
F	0.61427900	2.79449500	3.04298300
F	1.43343300	1.12679600	4.17835300
F	-0.64775300	1.69323400	4.43502800
C	2.76843500	-4.55027600	-1.27360100
C	3.21319100	-3.54088200	-2.14069100
C	3.43127900	-5.79011000	-1.33670800
C	4.26604300	-3.76357400	-3.03352200
H	2.75887800	-2.55706500	-2.14093200
C	4.48047000	-6.01554000	-2.22464900
H	3.12520100	-6.60529000	-0.68718300
C	4.90420700	-4.99979900	-3.08330700
H	4.58775000	-2.95371100	-3.68140700
H	4.96444700	-6.98863100	-2.24550100
H	5.72040300	-5.17203500	-3.77979500
C	2.14321800	-4.58964700	1.15638000
H	2.75729500	-5.49807400	1.13140200
H	2.83623700	-3.76658900	1.36692000
C	1.18359400	-4.74092100	2.31192100
C	1.07756800	-3.89232300	3.33933500
H	1.66136100	-2.97721300	3.39654400
H	0.39842200	-4.08559600	4.16601500
H	0.58652700	-5.65274100	2.32668500
H	-0.99492400	-5.37849100	0.92665200

INT-12-1

0 imaginary frequency

H = -5236.811538

G = -5237.007330

E(M06-2X-DCM) = -5237.654220

E(M06-2X-cyclohexane) = -5237.628983

C	-0.85055700	5.32143900	-0.43496100
C	-2.15673000	5.80021700	0.27341100
H	-1.89244100	6.48322400	1.08849600
H	-2.69006500	6.41129500	-0.47091400
C	-3.13661500	4.77605100	0.78828900
C	-1.17938900	4.35321000	-1.61123800
H	-0.33221000	4.32715100	-2.30898500
H	-2.04005900	4.72923000	-2.16755500
N	-1.48893000	2.98668700	-1.21695500
C	-2.53744500	2.25652300	-1.67603100
N	-2.45040200	0.93278300	-1.29698700
C	-3.38558500	-0.10251600	-1.43854800
C	-4.77534700	0.09298600	-1.38805600
C	-2.88919600	-1.40792000	-1.56360100
C	-5.63269300	-0.99930700	-1.49504200
C	-3.76413400	-2.48965300	-1.66128700
H	-1.81741500	-1.57584100	-1.58222100
C	-5.14379700	-2.29838400	-1.64215700
H	-5.82189800	-3.13778400	-1.73774600
C	-3.21032400	-3.88438100	-1.70579600
C	-7.11777000	-0.79323700	-1.35253800
F	-2.02271300	-3.94468200	-2.35457100
F	-4.04574600	-4.75328000	-2.30853800
F	-2.98375100	-4.37074200	-0.45137100
F	-7.50142500	0.44998500	-1.69631100
F	-7.51971500	-0.98947900	-0.06741500
F	-7.81954700	-1.66583400	-2.10941300
S	-3.78775200	2.90169000	-2.61357300
H	-5.17567600	1.08938800	-1.27292600
C	-3.61247500	4.74623000	2.03466300
H	-1.53462500	0.63329100	-0.95827000
H	-4.36479800	4.02338400	2.33902200
H	-0.74873300	2.48545200	-0.73240900
H	1.85345900	1.22585200	1.69335400
O	0.12588300	-1.57576000	0.91382100
O	2.31465000	-1.30827700	-0.44049700
P	1.14672000	-0.48929700	0.30678800

O	0.36946600	0.52060700	-0.45215100
C	1.47148200	-4.24028500	3.84838800
C	1.79033100	-4.45236900	2.51219500
C	1.24438400	-3.63731800	1.50747300
C	0.12684500	-2.29541700	3.22427900
C	0.60906900	-3.19708400	4.18682600
C	2.00257100	-2.20190700	-1.49157000
C	1.58519700	-3.49317200	-1.17810500
C	1.18093200	-4.33585100	-2.22851100
C	1.27425000	-3.92433300	-3.55300600
C	1.77301600	-2.65449200	-3.83855400
C	2.13612800	-1.75816800	-2.82087100
H	0.32070100	-3.04672700	5.22276200
H	1.87010400	-2.32696900	-4.86931600
C	1.53654600	-4.25794600	0.14375200
C	2.89075600	-4.97491200	0.45872400
H	3.11727600	-5.77168100	-0.25655200
H	3.70017700	-4.23734000	0.41436800
H	-0.27514000	-5.94941500	-2.18939400
H	1.37847500	-6.45607800	-1.83973400
C	0.50736000	-2.52236600	1.88824300
H	1.88234400	-4.88013400	4.62503500
H	0.96129700	-4.58203800	-4.35955000
C	2.72458700	-5.48029800	1.91026100
H	2.28972900	-6.48873200	1.93844400
H	3.67801000	-5.53269900	2.44741400
C	0.65144100	-5.64535100	-1.69260800
C	0.44424200	-5.33060200	-0.19861300
H	0.51448000	-6.21138200	0.44587000
H	-0.54709100	-4.89066400	-0.05536200
C	2.66813900	-0.40776900	-3.19338800
C	4.06235700	-0.16827500	-3.13215700
C	1.79367800	0.58522700	-3.69478000
C	5.00545300	-1.16978400	-2.73636500
C	4.58141100	1.12400200	-3.51868400
C	2.32958500	1.86701600	-4.09711300
C	6.35057700	-0.90851200	-2.69738800
H	4.64118200	-2.15576800	-2.46941200
C	5.98962200	1.36113100	-3.44646900
C	3.70111700	2.10671300	-3.98014000
C	6.85319200	0.37695500	-3.04687100
H	7.04377000	-1.69004300	-2.39797600
H	6.36080200	2.34295500	-3.73083900
H	4.09759000	3.07504100	-4.27941200

H	7.92207600	0.56723100	-3.00442100
C	-0.77873200	-1.17375300	3.62719200
C	-2.13038200	-1.17709800	3.19740000
C	-0.30703000	-0.14968600	4.48646900
C	-2.68865700	-2.21458300	2.38426600
C	-3.01242600	-0.10749700	3.60720500
C	-1.20799600	0.90268600	4.90265600
C	-3.99857200	-2.18167900	1.98344400
H	-2.06300800	-3.04698000	2.08339500
C	-4.36869000	-0.10318300	3.15321700
C	-2.52763200	0.90005800	4.44505500
C	-4.85257000	-1.10595400	2.35754600
H	-4.38528600	-2.98331500	1.36283300
H	-5.00881100	0.72151300	3.45777400
H	-3.19689800	1.70106500	4.75233700
H	-5.87657500	-1.08380200	1.99730300
C	-0.43033200	1.35284800	-4.36023200
H	-1.49719000	1.17648300	-4.45931400
C	0.38336000	0.38020500	-3.84107400
H	-0.04078600	-0.57125300	-3.54055900
C	0.10452800	2.61199700	-4.75851700
H	-0.56009100	3.36833100	-5.16593400
C	1.44411100	2.86012500	-4.62344400
H	1.86629700	3.81496400	-4.92870800
C	1.46379300	0.91494500	5.79660700
H	2.49727600	0.93586100	6.12968600
C	0.56672400	1.93753800	6.21721500
H	0.91598000	2.72016800	6.88540800
C	-0.72961200	1.92933100	5.77620500
H	-1.42672600	2.70461600	6.08573500
C	1.04234900	-0.08971600	4.96453700
H	1.74317200	-0.85679600	4.65717900
N	2.08341400	0.24248000	1.51641500
S	3.54475000	-0.19815100	2.23671300
C	4.85210200	0.00211000	0.87919300
O	3.53300100	-1.61251300	2.57381100
O	3.83065700	0.85057500	3.20768500
F	5.08094100	-1.17174900	0.30615800
F	4.44751900	0.89288800	-0.02646100
F	5.96585800	0.43667000	1.46488700
H	-3.53106100	4.07404800	0.05785300
H	-3.27854300	5.44713700	2.79886900
C	0.18896200	4.69507000	0.51012400
C	0.01020600	4.62040200	1.89885200

C	1.39538100	4.19606800	-0.01427000
C	0.99590900	4.08833800	2.73188600
H	-0.91328400	4.96425300	2.34491000
C	2.38898200	3.67221800	0.81310800
H	1.57476000	4.21657300	-1.08585900
C	2.19759900	3.62051400	2.19782600
H	0.82070400	4.03385100	3.80263500
H	3.31179100	3.30225100	0.37397200
H	2.97102100	3.22290800	2.84819500
C	-0.20881000	6.58265600	-1.12324400
H	0.70813500	6.27391500	-1.63726500
H	-0.90863200	6.91732900	-1.90399300
C	0.10630700	7.74143600	-0.21590300
H	-0.74387200	8.28272300	0.19838500
C	1.33790400	8.15051300	0.09160300
H	2.22163800	7.64906200	-0.29743600
H	1.51138800	9.00102800	0.74558400

INT-12-2

0 imaginary frequency

H = -5236.813701

G = -5237.008911

E(M06-2X-DCM) = -5237.657575

E(M06-2X-cyclohexane) = -5237.633088

C	-0.78277600	5.22403600	0.42919800
C	-2.09924400	5.20574700	1.26970100
H	-1.96945100	5.90504600	2.10934200
H	-2.89543500	5.63556300	0.65043000
C	-2.56721100	3.88056900	1.81524500
C	-1.03052200	4.54769600	-0.94402400
H	-0.17052500	4.69899000	-1.60558600
H	-1.88419900	5.02971600	-1.42376300
N	-1.33798800	3.12915900	-0.87215500
C	-2.44800000	2.53429600	-1.37306800
N	-2.41525100	1.16504400	-1.19172500
C	-3.39509900	0.19365400	-1.42938400
C	-4.77639600	0.43586900	-1.34591800
C	-2.95221900	-1.11164800	-1.69167400
C	-5.67532200	-0.60832600	-1.55000300
C	-3.86836800	-2.14440500	-1.88654000
H	-1.88789700	-1.31777300	-1.74076100
C	-5.23954600	-1.90445400	-1.83094300
H	-5.95080400	-2.70367300	-2.00085300
C	-3.36739600	-3.54640000	-2.07898800

C	-7.15006400	-0.36329300	-1.36792900
F	-4.24168300	-4.32067200	-2.75142500
F	-3.14184800	-4.16481400	-0.88345100
F	-2.19076900	-3.58400500	-2.74989600
F	-7.49005200	0.92226500	-1.57433000
F	-7.54813200	-0.67936400	-0.10554000
F	-7.89159200	-1.12491800	-2.20328500
S	-3.68940700	3.36568800	-2.16028800
H	-5.13458000	1.43108300	-1.12757700
C	-3.82529200	3.44258300	1.74203500
H	-1.51178100	0.78675200	-0.90659800
H	-4.12101700	2.49189800	2.17708900
H	-0.62043000	2.52378700	-0.48409200
H	1.93188700	1.04792100	1.77571100
O	0.08922700	-1.61664400	0.76428000
O	2.28799400	-1.30152200	-0.56175600
P	1.15014900	-0.51654900	0.26238100
O	0.41252300	0.59098200	-0.39239700
C	1.33450300	-4.62918600	3.38976600
C	1.64547500	-4.70933900	2.03728100
C	1.13051900	-3.77260400	1.12648100
C	0.05722000	-2.58508300	2.98006400
C	0.50768900	-3.59951500	3.84000100
C	1.94185100	-2.06163200	-1.70399000
C	1.47401400	-3.36097700	-1.52992300
C	1.03506600	-4.06854000	-2.66266800
C	1.14410200	-3.51925400	-3.93517300
C	1.69252600	-2.24602000	-4.08408800
C	2.09105600	-1.48019800	-2.97719800
H	0.22274200	-3.55105600	4.88662300
H	1.80071500	-1.81244000	-5.07379000
C	1.39591400	-4.25832300	-0.29666500
C	2.72080600	-5.05731400	-0.06617200
H	2.91355300	-5.78345700	-0.86194200
H	3.55918800	-4.35183000	-0.03925500
H	-0.48541300	-5.61738800	-2.78704700
H	1.14690800	-6.22462800	-2.50314500
C	0.43437600	-2.67864300	1.62757600
H	1.72225000	-5.36226200	4.09235000
H	0.80447900	-4.07230100	-4.80684700
C	2.53784000	-5.70408500	1.32586000
H	2.06363200	-6.69221000	1.25160500
H	3.48948400	-5.84953200	1.84889400
C	0.45361300	-5.40562000	-2.26641100

C	0.26097900	-5.24412000	-0.74580700
H	0.29620500	-6.19085800	-0.19939200
H	-0.71201600	-4.78299400	-0.55170400
C	2.66974400	-0.11532200	-3.19346300
C	4.07035200	0.06905900	-3.09971100
C	1.82944500	0.96119800	-3.56401800
C	4.97867600	-1.00456600	-2.83205600
C	4.63192500	1.38332300	-3.31405900
C	2.40661400	2.26870000	-3.78696200
C	6.33108500	-0.79362400	-2.75610400
H	4.58180300	-2.00461700	-2.69546100
C	6.04649100	1.56374300	-3.20898600
C	3.78474800	2.44653900	-3.63916400
C	6.87613700	0.50930400	-2.93697500
H	6.99745500	-1.62890000	-2.55788600
H	6.45020600	2.56163400	-3.36344400
H	4.21211700	3.43392400	-3.80269000
H	7.95018800	0.65828100	-2.86798600
C	-0.81883800	-1.48865200	3.50163800
C	-2.17472200	-1.42292500	3.09050800
C	-0.31629700	-0.56488900	4.45158800
C	-2.75907400	-2.35371000	2.17319600
C	-3.03351100	-0.39092200	3.62680200
C	-1.19006700	0.45850800	4.98240900
C	-4.07239000	-2.25597800	1.79415900
H	-2.15000300	-3.15521600	1.77146600
C	-4.39779900	-0.32225700	3.20154400
C	-2.51831200	0.51977900	4.55347900
C	-4.90619200	-1.22054800	2.30254800
H	-4.47752300	-2.97428000	1.08908500
H	-5.02424600	0.46576300	3.61308100
H	-3.16967100	1.29404200	4.95380700
H	-5.93443800	-1.14366800	1.96240000
C	-0.36607900	1.88198500	-4.11908300
H	-1.43716500	1.75399400	-4.24344100
C	0.41476200	0.82139300	-3.74112700
H	-0.03963600	-0.14928600	-3.57721500
C	0.20754300	3.16865600	-4.33147300
H	-0.43299900	3.99651400	-4.62092400
C	1.55361100	3.35369800	-4.16495000
H	2.00415700	4.33028300	-4.32605200
C	1.49414800	0.33483600	5.82821400
H	2.53223400	0.30342500	6.14581700
C	0.62587600	1.33275200	6.35447900

H	1.00262400	2.04517900	7.08347600
C	-0.67692600	1.39009900	5.93873000
H	-1.35232100	2.14778900	6.32917700
C	1.03976100	-0.57960200	4.91360200
H	1.71838200	-1.33021800	4.52612800
N	2.11288500	0.07051800	1.53088100
S	3.54975400	-0.48321100	2.22301100
C	4.87460200	-0.26056700	0.88670300
O	3.47021200	-1.91445000	2.46708000
O	3.87664400	0.48994400	3.25750900
F	5.02759100	-1.39266000	0.21341800
F	4.53762400	0.73102700	0.06101600
F	6.01132600	0.04513600	1.50870800
H	-1.82738400	3.27592800	2.33911500
H	-4.59852800	4.00404400	1.22278900
C	0.40920100	4.61621700	1.19235000
C	0.53190800	4.77891500	2.58460100
C	1.45174000	3.94355000	0.53426800
C	1.62590500	4.27884000	3.28855000
H	-0.24354800	5.29789900	3.13848500
C	2.55956500	3.45170100	1.23345400
H	1.42233400	3.79812300	-0.54071700
C	2.65110000	3.60913600	2.61745100
H	1.67503200	4.40900200	4.36610000
H	3.35282800	2.94978500	0.68591200
H	3.50218500	3.21270600	3.16218300
C	-0.47631600	6.73907400	0.14320000
H	-1.36054700	7.18232000	-0.33336900
H	-0.36209100	7.23367000	1.11858200
C	0.73942600	7.03231700	-0.69319900
H	1.69453600	6.69896700	-0.28797200
C	0.72167700	7.68236100	-1.85871000
H	-0.20592200	8.03859900	-2.30284000
H	1.63445000	7.89153300	-2.41071700

INT-12-3

0 imaginary frequency

H = -5236.813582

G = -5237.008796

E(M06-2X-DCM) = -5237.659189

E(M06-2X-cyclohexane) = -5237.634542

C	-1.17206900	5.06872400	0.24750100
C	-2.29660700	4.99255700	1.32066200
H	-1.95707900	5.56100600	2.19991600

H	-3.15766900	5.54726300	0.93366300
C	-2.76299100	3.62695200	1.75821100
C	-1.63318500	4.37397100	-1.06279400
H	-0.97197000	4.65471300	-1.89433000
H	-2.63377600	4.71719900	-1.32714000
N	-1.70399800	2.92680800	-0.96729200
C	-2.72684300	2.16898800	-1.43415100
N	-2.51730500	0.82323500	-1.20314000
C	-3.36274100	-0.27263600	-1.41940000
C	-4.76475400	-0.20333500	-1.35740100
C	-2.75687100	-1.51911500	-1.63774800
C	-5.52409600	-1.35563800	-1.54592900
C	-3.53511900	-2.66258600	-1.81458700
H	-1.67460500	-1.59292500	-1.66658100
C	-4.92621400	-2.59381800	-1.78525800
H	-5.52947400	-3.47965000	-1.94313600
C	-2.86316400	-3.99698700	-1.95808200
C	-7.02108900	-1.29074900	-1.39438300
F	-2.59093800	-4.55176800	-0.74146000
F	-1.67657000	-3.90772900	-2.60603900
F	-3.62179900	-4.88960900	-2.62453100
F	-7.51255400	-0.06179600	-1.63611400
F	-7.40277400	-1.62759500	-0.13209100
F	-7.64630100	-2.15553900	-2.22449700
S	-4.06908800	2.80698800	-2.23597600
H	-5.24753400	0.74415500	-1.16949000
C	-4.04209400	3.24732400	1.77446800
H	-1.57692200	0.57549000	-0.89413100
H	-4.33645100	2.25874200	2.11603400
H	-0.88393800	2.44742700	-0.60520600
H	1.81568500	1.32220200	1.77706700
O	0.27417400	-1.55773800	0.82810400
O	2.43877300	-1.03645200	-0.48664900
P	1.21189400	-0.35846500	0.30551300
O	0.36129200	0.63955800	-0.38672700
C	1.81404500	-4.29141900	3.59654800
C	2.15478300	-4.39170100	2.25261900
C	1.54919800	-3.56107100	1.29581300
C	0.31632000	-2.42890200	3.08344000
C	0.86637700	-3.34638900	3.99236000
C	2.19484000	-1.87810700	-1.59632100
C	1.88516100	-3.21693100	-1.37130400
C	1.54929700	-4.01715300	-2.47740200
C	1.60289900	-3.50963600	-3.77058900

C	1. 99284400	-2. 18587200	-3. 96855400
C	2. 28574200	-1. 33448300	-2. 89159800
H	0. 56126000	-3. 28694200	5. 03279100
H	2. 05782600	-1. 78229800	-4. 97459800
C	1. 89748900	-4. 06737200	-0. 10190300
C	3. 30471000	-4. 68936800	0. 18049500
H	3. 59927200	-5. 41782600	-0. 58134200
H	4. 05104600	-3. 88684600	0. 19088800
H	0. 23468800	-5. 74695900	-2. 55277800
H	1. 92540300	-6. 13397300	-2. 22797000
C	0. 72302600	-2. 53603400	1. 74034800
H	2. 27351200	-4. 94311000	4. 33517700
H	1. 34230500	-4. 13457900	-4. 62061200
C	3. 17383200	-5. 29853600	1. 59568500
H	2. 82411700	-6. 33914300	1. 55550900
H	4. 12576500	-5. 30630000	2. 13793400
C	1. 13218300	-5. 39916200	-2. 03204200
C	0. 89891500	-5. 20244300	-0. 52163700
H	1. 04234500	-6. 11521800	0. 06344600
H	-0. 12597000	-4. 85778000	-0. 35581700
C	2. 70737400	0. 07736600	-3. 16577900
C	4. 07881100	0. 42004900	-3. 08425500
C	1. 75474100	1. 03514000	-3. 58707000
C	5. 09842700	-0. 53042000	-2. 75810100
C	4. 49395800	1. 77403100	-3. 37297500
C	2. 18635500	2. 38248300	-3. 88803100
C	6. 41904100	-0. 16818400	-2. 69576500
H	4. 81319600	-1. 55847500	-2. 56373800
C	5. 87996800	2. 11408100	-3. 28206400
C	3. 53679800	2. 71775000	-3. 75777200
C	6. 81885600	1. 17413000	-2. 95193500
H	7. 17193500	-0. 91250100	-2. 45064200
H	6. 17270800	3. 13966900	-3. 49458200
H	3. 85535200	3. 73337400	-3. 98503200
H	7. 86980800	1. 44362500	-2. 89374100
C	-0. 68769400	-1. 41575500	3. 53889100
C	-2. 03531800	-1. 53089200	3. 11271400
C	-0. 30805600	-0. 38209500	4. 43071700
C	-2. 49570700	-2. 58165700	2. 25635600
C	-3. 01260300	-0. 56739500	3. 56730200
C	-1. 29804700	0. 57381000	4. 87693300
C	-3. 80537200	-2. 65939200	1. 86061600
H	-1. 79323800	-3. 33399100	1. 91656400
C	-4. 36839000	-0. 68178400	3. 12537100

C	-2.61708700	0.45828000	4.43059400
C	-4.75815000	-1.69221200	2.28835900
H	-4.11592500	-3.46482700	1.20306700
H	-5.08566800	0.05782700	3.47354400
H	-3.35526900	1.18442200	4.76453900
H	-5.78283900	-1.75556100	1.93539400
C	-0.52992100	1.68110400	-4.17155200
H	-1.58152300	1.43162800	-4.27656800
C	0.36280800	0.73415200	-3.74260500
H	0.01669000	-0.26883300	-3.51954200
C	-0.09814500	3.00619700	-4.46769000
H	-0.82406800	3.74008300	-4.80574200
C	1.22104100	3.34387100	-4.32579600
H	1.56568300	4.34941600	-4.55683000
C	1.36695800	0.80281500	5.76241300
H	2.39532500	0.90473300	6.09617500
C	0.38666800	1.73779000	6.20107800
H	0.67002800	2.53761600	6.87997200
C	-0.90670200	1.62302100	5.76691300
H	-1.66722400	2.32867800	6.09299700
C	1.03135000	-0.21818300	4.91119000
H	1.79312200	-0.91855300	4.58985200
N	2.09054300	0.35844500	1.56697400
S	3.57673600	-0.02401100	2.27142000
C	4.87643700	0.33124000	0.93637100
O	3.65485600	-1.45270400	2.53066400
O	3.78881200	0.98704600	3.29956600
F	5.95528500	0.80705400	1.55630300
F	5.18696600	-0.79367700	0.30558600
F	4.42209000	1.23978700	0.07490900
H	-2.00556200	2.92752700	2.11023100
H	-4.83897200	3.89978100	1.42440500
C	0.18378100	4.51811700	0.73283000
C	0.46421000	4.27399200	2.08620800
C	1.23142800	4.32202900	-0.18695000
C	1.73477500	3.86645400	2.50588600
H	-0.30600800	4.40217900	2.83784400
C	2.50116400	3.92093100	0.22377300
H	1.06124000	4.48244000	-1.24737000
C	2.76444000	3.69984000	1.57770800
H	1.91695300	3.68162800	3.56106200
H	3.28178600	3.77411700	-0.51731600
H	3.75260800	3.39487800	1.90791200
C	-0.92501500	6.58860900	-0.08076800

H	-0.56964800	7.07722400	0.83470000
H	-0.09611400	6.64150700	-0.80043900
C	-2.09905700	7.35377600	-0.63310800
H	-2.48827200	7.02653500	-1.59744900
C	-2.66282300	8.40855000	-0.04142100
H	-2.30941100	8.78318800	0.91750200
H	-3.49467500	8.94181800	-0.49380900

INT-12-4

0 imaginary frequency

H = -5236.804627

G = -5237.002441

E(M06-2X-DCM) = -5237.647830

E(M06-2X-cyclohexane) = -5237.621621

C	0.58842300	5.12683600	0.93966900
C	-0.39846300	5.14972800	2.15180800
H	0.10444600	5.66786000	2.98204300
H	-1.24736600	5.78764400	1.87794200
C	-0.92126800	3.83056800	2.65888000
C	-0.18519800	4.75742200	-0.35080000
H	0.46097800	4.86046200	-1.22990300
H	-1.01300400	5.45700400	-0.48173900
N	-0.76334400	3.42427700	-0.34656300
C	-2.05356000	3.12643400	-0.63318300
N	-2.27939600	1.76386300	-0.60524800
C	-3.45838700	1.03679800	-0.81499400
C	-4.73581000	1.49448500	-0.45102800
C	-3.33073800	-0.24946000	-1.36068300
C	-5.84796200	0.68407400	-0.66697000
C	-4.45593200	-1.04834000	-1.56282800
H	-2.34817400	-0.62230700	-1.63130800
C	-5.72795300	-0.58723800	-1.23132100
H	-6.60394200	-1.19967900	-1.40799800
C	-4.28462400	-2.44738700	-2.08073100
C	-7.20454200	1.14217800	-0.20024200
F	-3.24989600	-2.55127100	-2.94802100
F	-5.38685200	-2.90371800	-2.70797800
F	-4.02184800	-3.32805200	-1.07128600
F	-8.18628600	0.72719100	-1.03205400
F	-7.29194100	2.48080400	-0.09781200
F	-7.50110900	0.63168400	1.02625900
S	-3.22499500	4.28452900	-1.00925300
H	-4.84934000	2.47455100	-0.01192400
C	-2.20661100	3.57684300	2.91036100

H	-1.44034400	1.18809100	-0.53773000
H	-2.52751700	2.61729900	3.30592400
H	-0.12635100	2.64783200	-0.19258900
H	2.47777800	0.30775800	1.37100700
O	-0.11508800	-1.70022200	0.49921800
O	1.79695200	-1.53478200	-1.23861000
P	1.05137000	-0.74372500	-0.06186200
O	0.46900900	0.59100600	-0.34167500
C	0.92788500	-5.27644500	2.39718800
C	1.00551900	-5.17480500	1.01261800
C	0.53267900	-4.02897200	0.35110800
C	-0.02140800	-3.02499300	2.51720600
C	0.36798700	-4.22773600	3.12929700
C	1.10598300	-2.03883400	-2.35735500
C	0.45802400	-3.26450600	-2.25214900
C	-0.29780500	-3.71027800	-3.34985400
C	-0.31977400	-2.99218200	-4.54073300
C	0.40910300	-1.80720600	-4.63935500
C	1.12588000	-1.29144600	-3.54796400
H	0.24560100	-4.32208400	4.20406400
H	0.41369600	-1.24711900	-5.56958400
C	0.44454100	-4.31823600	-1.14734800
C	1.61426900	-5.34589000	-1.29282400
H	1.51932800	-5.95940000	-2.19395900
H	2.56096500	-4.79809700	-1.34972500
H	-2.07480000	-4.96214000	-3.34718200
H	-0.55936400	-5.85740700	-3.47391900
C	0.14167200	-2.93849500	1.12063100
H	1.27921500	-6.16930500	2.90797300
H	-0.90205100	-3.34550400	-5.38755800
C	1.56484500	-6.16793400	0.01595400
H	0.91442500	-7.04762700	-0.08316100
H	2.55192900	-6.53781800	0.31486000
C	-1.03478200	-4.98387100	-3.00672100
C	-0.91909500	-5.02654100	-1.46977100
H	-0.96861500	-6.03791700	-1.05645100
H	-1.73697300	-4.44534900	-1.03230900
C	1.88315500	-0.00783700	-3.67979900
C	3.29941400	-0.02824200	-3.69870500
C	1.18071800	1.21200000	-3.83234200
C	4.06255200	-1.23530700	-3.59676800
C	4.02648800	1.21153700	-3.85041400
C	1.92244900	2.44265800	-3.99701800
C	5.43248100	-1.21725900	-3.61798000

H	3.54090600	-2.18168000	-3.50674400
C	5.45630300	1.18662600	-3.86368600
C	3.31964000	2.40908300	-3.99450600
C	6.14344400	0.00904200	-3.74746900
H	5.98516100	-2.14907700	-3.53577100
H	5.98555800	2.13028100	-3.97310100
H	3.87204400	3.33887200	-4.11536900
H	7.22981200	0.00297500	-3.75829800
C	-0.64299100	-1.92851800	3.32735300
C	-2.00827100	-1.59894600	3.12363100
C	0.09909000	-1.27606300	4.34315100
C	-2.83928600	-2.26091700	2.16436200
C	-2.62158400	-0.56770100	3.93114500
C	-0.53212400	-0.25693000	5.15154000
C	-4.15311800	-1.91106700	1.99251000
H	-2.42180700	-3.06161000	1.56500500
C	-3.99270400	-0.22473400	3.71095000
C	-1.86886500	0.07375700	4.91874800
C	-4.74049800	-0.86859800	2.76304100
H	-4.74916100	-2.43091500	1.25006400
H	-4.42782500	0.56514700	4.31865500
H	-2.33848100	0.84449800	5.52645100
H	-5.77216900	-0.58253000	2.58317200
C	-0.89593500	2.49726000	-3.97118800
H	-1.98065300	2.53811700	-3.94285500
C	-0.24972700	1.29822600	-3.81908300
H	-0.82889700	0.39133000	-3.68537900
C	-0.15964600	3.70394900	-4.14611300
H	-0.69337600	4.64263000	-4.26196000
C	1.20901500	3.67297200	-4.15690100
H	1.78478800	4.58611000	-4.29008700
C	2.16318900	-0.93081300	5.60786400
H	3.20582100	-1.18035400	5.78454100
C	1.53350100	0.06504300	6.40665200
H	2.09578100	0.56289000	7.19187400
C	0.22436000	0.39169800	6.17752500
H	-0.27051200	1.15362100	6.77498600
C	1.47220600	-1.57290600	4.61334400
H	1.96722500	-2.32326500	4.01239300
N	2.35886200	-0.65596200	1.04270500
S	3.89426900	-1.37573000	0.77580900
C	4.58105000	-1.31817900	2.53105100
O	4.75309800	-0.47949200	0.01239400
O	3.71806400	-2.77972000	0.44109000

F	4.19131200	-0.20014800	3.14906500
F	4.18258500	-2.38181900	3.22295400
F	5.90742700	-1.33069500	2.43078700
H	-0.17914500	3.06168300	2.87275900
H	-2.98559600	4.30834000	2.70668900
C	1.80832700	4.22267900	1.19200900
C	2.40884600	4.17189500	2.46333500
C	2.41450100	3.47848000	0.16824000
C	3.54982600	3.40803200	2.70398700
H	1.98261600	4.73693700	3.28652500
C	3.55899000	2.70941900	0.40084800
H	2.00813000	3.48785000	-0.83720400
C	4.13382100	2.66962500	1.67161700
H	3.98414400	3.39310700	3.70038400
H	4.00300700	2.14854600	-0.41655000
H	5.02841700	2.08030300	1.84992800
C	1.09677700	6.60859100	0.77556200
H	0.20694600	7.25393100	0.73483500
H	1.63935500	6.87592300	1.68996400
C	1.96774700	6.90085800	-0.41696400
H	1.47684500	6.91101500	-1.39021900
C	3.27322000	7.16816100	-0.35623700
H	3.81121400	7.17808500	0.58948000
H	3.85519100	7.38735800	-1.24764000

INT-12-5

0 imaginary frequency

H = -5236.799009

G = -5236.997869

E(M06-2X-DCM) = -5237.656333

E(M06-2X-cyclohexane) = -5237.626766

O	-0.82165700	-2.39732900	0.08896000
O	-2.76546400	-0.68254400	0.09782400
P	-1.13633200	-0.79115800	0.22531100
O	-0.54276500	-0.00032000	-0.90053200
C	-1.80155700	-4.15993600	-3.58169100
C	-2.76196900	-4.00631600	-2.58697300
C	-2.40942800	-3.49108500	-1.33122500
C	-0.10551700	-3.21712100	-2.08516900
C	-0.48259500	-3.79841400	-3.30917200
C	-3.58312500	-1.35809400	1.01024300
C	-3.83367300	-2.71884500	0.82814000
C	-4.51725600	-3.42873600	1.82838300
C	-5.04007700	-2.77189400	2.93627900

C	-4.88776600	-1.38995800	3.03437500
C	-4.15494800	-0.65376700	2.08830700
H	0.28412800	-3.94926400	-4.06326400
H	-5.32730100	-0.85492500	3.87092800
C	-3.57535100	-3.63873200	-0.36246100
C	-4.77572400	-3.61699200	-1.36875000
H	-5.01907700	-2.57384500	-1.60359000
H	-5.67615200	-4.08255000	-0.95620300
H	-5.56251300	-5.21203200	1.17006800
H	-4.31166700	-5.53248000	2.36652400
C	-1.11113600	-3.03284600	-1.11697200
H	-2.06537800	-4.56958200	-4.55365900
H	-5.57211300	-3.32034300	3.70956700
C	-4.24075600	-4.32669400	-2.63226500
H	-4.72143200	-3.97371700	-3.55213200
H	-4.41421700	-5.41097100	-2.58493600
C	-4.56059100	-4.90563700	1.50260300
C	-3.52746700	-5.02586800	0.36283500
H	-2.52578900	-5.16574800	0.78507700
H	-3.72287100	-5.86042700	-0.31789900
C	-4.08789700	0.83335500	2.24316200
C	-3.41944000	1.40434000	3.35286600
C	-4.81022100	1.65893300	1.34534100
C	-2.64674200	0.62733500	4.27431100
C	-3.49316000	2.83092500	3.57536400
C	-4.85747000	3.08615900	1.56930700
C	-2.01561000	1.20918300	5.34149600
H	-2.53000600	-0.43327400	4.09346400
C	-2.82984900	3.39617300	4.70957800
C	-4.20697900	3.63025500	2.67970700
C	-2.11527400	2.61063200	5.57222600
H	-1.41113500	0.59793600	6.00518800
H	-2.90327000	4.47014600	4.86541600
H	-4.25625700	4.70404500	2.84929900
H	-1.60877900	3.05248200	6.42618600
C	1.33506000	-2.88240800	-1.86102200
C	1.97737900	-1.94031700	-2.70241000
C	2.08599700	-3.59371400	-0.89092900
C	1.26685900	-1.13786400	-3.65459400
C	3.40801800	-1.75434900	-2.60799900
C	3.50574700	-3.35126300	-0.76868200
C	1.92338400	-0.26792400	-4.48710500
H	0.18658600	-1.21017500	-3.69876300
C	4.05803800	-0.85530400	-3.51365400

C	4. 13090500	-2. 45347400	-1. 63810500
C	3. 34078700	-0. 13527500	-4. 43243100
H	1. 35273700	0. 32724100	-5. 19427400
H	5. 14006300	-0. 76176800	-3. 45372200
H	5. 20312700	-2. 29035100	-1. 55437800
H	3. 84747300	0. 53845800	-5. 11891300
C	-6. 22658600	1. 97027600	-0. 62638400
H	-6. 76997700	1. 54804500	-1. 46774300
C	-5. 53771600	1. 14358200	0. 22375700
H	-5. 54872600	0. 07279300	0. 05454400
C	-6. 24748700	3. 37826800	-0. 41418500
H	-6. 79575300	4. 01945100	-1. 09898900
C	-5. 58464700	3. 91380800	0. 65741100
H	-5. 60119300	4. 98588300	0. 83996200
C	2. 26304900	-5. 23913100	0. 90810100
H	1. 79462600	-5. 97625200	1. 55466900
C	3. 65484500	-4. 97370400	1. 04299600
H	4. 23472400	-5. 50411000	1. 79339800
C	4. 25554200	-4. 05964300	0. 22136500
H	5. 32051400	-3. 85504700	0. 30233700
C	1. 50997300	-4. 57908200	-0. 02696600
H	0. 45443400	-4. 80513900	-0. 11805100
C	-1. 43949800	3. 27273100	-2. 66893000
C	-2. 06208600	3. 22641200	-1. 24098000
H	-3. 15256600	3. 28073900	-1. 34772500
H	-1. 83967000	2. 26279500	-0. 77480500
C	-1. 61084200	4. 32918700	-0. 31741100
C	0. 10353000	3. 36909500	-2. 55620500
H	0. 34278900	4. 32210100	-2. 07438300
H	0. 55757800	3. 36744000	-3. 55366700
N	0. 71781000	2. 29890500	-1. 75497500
C	1. 93098300	2. 39084100	-1. 24167500
N	2. 42587800	1. 44372300	-0. 43556100
C	3. 74314400	1. 40572400	0. 12568200
C	3. 90298300	1. 55406900	1. 50770400
C	4. 84165800	1. 15261700	-0. 69528200
C	5. 18301100	1. 46171100	2. 05407500
C	6. 11686100	1. 06753500	-0. 13170300
H	4. 69245200	1. 00355300	-1. 75945800
C	6. 29357600	1. 22189700	1. 24128800
H	7. 28356800	1. 15797000	1. 67557500
C	7. 28325100	0. 78729800	-1. 04240500
C	5. 35946900	1. 57554900	3. 54958700
F	7. 38602000	1. 72556900	-2. 01064600

F	7.14020000	-0.40439900	-1.67726500
F	8.45444900	0.75156000	-0.38068600
F	5.15237000	0.39350200	4.16220900
F	4.49801700	2.46424700	4.08167900
F	6.61180800	1.97721500	3.86775900
S	2.86738400	3.84119900	-1.65994600
H	3.03643500	1.71722300	2.14076900
H	1.80994100	0.68243800	-0.10333200
H	0.17559000	1.43816400	-1.53890300
C	-0.96115100	4.13588200	0.83306700
H	-0.70609900	3.14287500	1.19795800
H	3.89404600	3.56466400	-0.83369300
H	-0.68809400	4.96843400	1.47672300
N	-0.80022200	-0.41315500	1.75881800
S	0.68238800	-0.31454500	2.30112400
O	0.90869500	0.88763200	3.11770400
O	1.72305700	-0.62031300	1.27908000
C	0.79775100	-1.74019600	3.50263100
F	0.57359300	-2.89787900	2.87706500
F	-0.10585500	-1.59502800	4.48301600
F	2.01921600	-1.76517100	4.04636900
C	-1.84722200	2.06011800	-3.53320600
C	-2.72852300	1.06918700	-3.08126500
C	-1.35198700	1.94085800	-4.84485000
C	-3.09066800	-0.00172300	-3.90301100
H	-3.13616600	1.10678700	-2.07929300
C	-1.71428400	0.87626600	-5.66852800
H	-0.67551800	2.69259500	-5.24431900
C	-2.58729400	-0.10668700	-5.19747900
H	-3.76315900	-0.76154900	-3.51511600
H	-1.31646300	0.81776500	-6.67854000
H	-2.86891500	-0.94188800	-5.83291900
C	-1.87802800	4.58897100	-3.40193100
H	-1.51872600	5.45770500	-2.83773600
H	-1.37001500	4.62466400	-4.37619400
C	-3.36049500	4.71836400	-3.62342400
C	-4.09747900	5.75780200	-3.22928500
H	-3.66473500	6.59988000	-2.69217900
H	-5.16343000	5.81149800	-3.43360700
H	-3.83779300	3.89819000	-4.15836600
H	-1.87016400	5.34845400	-0.60604300

INT-12-6

0 imaginary frequency

H = -5236.808738

G = -5237.004814

E(M06-2X-DCM) = -5237.654317

E(M06-2X-cyclohexane) = -5237.629096

C	0.32279100	5.07911100	0.79238000
C	-0.46489100	4.65058800	2.08210200
H	-0.05692800	5.21252200	2.93110300
H	-1.50328900	4.98303800	1.95971800
C	-0.46794900	3.18368800	2.43901400
C	-0.48051800	4.73289800	-0.48682500
H	0.10849800	5.00119600	-1.37506100
H	-1.37620700	5.35419400	-0.51335800
N	-0.93685100	3.35417900	-0.59026400
C	-2.16986200	2.98034300	-1.03351900
N	-2.30924700	1.60645600	-1.04772100
C	-3.39073400	0.78779000	-1.39771700
C	-4.74101400	1.16664200	-1.31928000
C	-3.07960800	-0.52542100	-1.78876400
C	-5.73606800	0.24931000	-1.65374800
C	-4.08950200	-1.42743100	-2.11500700
H	-2.04189100	-0.83914400	-1.83261900
C	-5.43014500	-1.04882700	-2.06308100
H	-6.21512300	-1.74474700	-2.33325200
C	-3.73106000	-2.84770800	-2.44643900
C	-7.18241600	0.63256200	-1.47900800
F	-4.65108100	-3.44158500	-3.23220800
F	-3.63036300	-3.61394800	-1.32139900
F	-2.53523800	-2.94433200	-3.07492200
F	-7.38022300	1.96006200	-1.57475200
F	-7.64716900	0.25045300	-0.25888000
F	-7.97445000	0.03102900	-2.39496300
S	-3.35617000	4.07666000	-1.51869100
H	-5.00033900	2.16784000	-1.00811300
C	0.26716700	2.63578300	3.41175100
H	-1.45458700	1.08460300	-0.85047400
H	0.18808800	1.58314900	3.66543800
H	-0.25132400	2.61971600	-0.43919000
H	1.71690700	0.79117200	1.84831500
O	-0.22162300	-1.69316600	0.69927700
O	2.02453800	-1.51605200	-0.58928200
P	0.93379400	-0.67083700	0.24071500
O	0.30155600	0.50068500	-0.41429600
C	0.69300100	-5.00421100	3.10247000
C	1.01714100	-5.00808100	1.75093500

C	0.60896000	-3.95741200	0.91407700
C	-0.38861900	-2.82381400	2.83940600
C	-0.04636900	-3.94210400	3.61941800
C	1.62340200	-2.15758700	-1.78835700
C	1.00735400	-3.40340800	-1.70700400
C	0.50074900	-3.98071300	-2.88393400
C	0.68607100	-3.36708600	-4.11693700
C	1.38353500	-2.16275200	-4.17732200
C	1.85656600	-1.52016400	-3.02100400
H	-0.35145400	-3.95192900	4.66114700
H	1.55642000	-1.68245000	-5.13564100
C	0.82217700	-4.36761100	-0.54002100
C	2.04966900	-5.32350300	-0.37816500
H	2.15793100	-6.00997400	-1.22352000
H	2.96165500	-4.71885800	-0.31360500
H	-1.19276100	-5.32295300	-3.11007200
H	0.35266800	-6.14094500	-2.87352100
C	0.01105100	-2.84078600	1.48985700
H	0.99436000	-5.82442000	3.74881700
H	0.29325600	-3.81729900	-5.02462600
C	1.80101100	-6.03930200	0.96814000
H	1.22498600	-6.96478900	0.83198600
H	2.73225900	-6.31948000	1.47295200
C	-0.23781600	-5.26254300	-2.57843100
C	-0.41745100	-5.18282700	-1.04992200
H	-0.49596000	-6.16117900	-0.56746300
H	-1.33080700	-4.62377100	-0.82367600
C	2.60637700	-0.23387200	-3.18537600
C	4.01911900	-0.23555600	-3.08894000
C	1.91575900	0.94123300	-3.56712600
C	4.77514100	-1.40743100	-2.76486500
C	4.75289100	0.97968700	-3.36181100
C	2.66305000	2.14778100	-3.84418100
C	6.14328500	-1.37583900	-2.68763400
H	4.24837900	-2.33718300	-2.58115400
C	6.17971500	0.97155900	-3.26338600
C	4.05639900	2.13414300	-3.73278100
C	6.85928400	-0.16984200	-2.93332800
H	6.69079700	-2.28125300	-2.44000700
H	6.71412400	1.89687100	-3.46519700
H	4.61391900	3.04385800	-3.94668900
H	7.94363700	-0.16389800	-2.86564400
C	-1.19038400	-1.72251100	3.45817900
C	-2.51207100	-1.47253900	3.00638500

C	-0.66916200	-1.00697400	4.56664500
C	-3.12506200	-2.19701400	1.93460700
C	-3.31076400	-0.46161700	3.66356400
C	-1.49748800	-0.03005200	5.23877000
C	-4.39930600	-1.91495500	1.51696400
H	-2.57155800	-2.98963200	1.44499700
C	-4.63032000	-0.18655800	3.18466500
C	-2.78660900	0.22177200	4.76354500
C	-5.16196300	-0.88372500	2.13424500
H	-4.82754700	-2.48171000	0.69714800
H	-5.20197000	0.59576900	3.67818300
H	-3.39855600	0.97015300	5.26281400
H	-6.15385900	-0.65143400	1.75848300
C	-0.14677100	2.15303400	-4.07347700
H	-1.22945700	2.17337200	-4.15672000
C	0.49026300	0.99885600	-3.69896900
H	-0.08969300	0.10648500	-3.49409600
C	0.59530000	3.33890400	-4.34420600
H	0.07009200	4.24306100	-4.63823000
C	1.95976300	3.33220900	-4.23179600
H	2.53867000	4.22951400	-4.43717000
C	1.13481500	-0.48038700	6.13337400
H	2.15731200	-0.62971400	6.46812700
C	0.30282900	0.45606000	6.80950100
H	0.68982900	1.00138500	7.66586800
C	-0.97425200	0.67425900	6.36819400
H	-1.61737200	1.39766300	6.86361200
C	0.66658800	-1.18701500	5.05539900
H	1.32100700	-1.88997100	4.55376000
N	1.89157500	-0.16985800	1.54333800
S	3.24205000	-0.84573300	2.29873700
C	4.63859000	-0.70912100	1.02319000
O	3.03816600	-2.27264400	2.49750200
O	3.57772700	0.07634900	3.37397300
F	5.76536100	-0.48980000	1.69864300
F	4.73873700	-1.84980300	0.35085300
F	4.41225800	0.30039100	0.18814700
H	-1.14818000	2.54789400	1.87664000
H	0.95318200	3.22463500	4.01621500
C	1.74840900	4.50120200	0.81324200
C	2.57427000	4.73045800	1.92938400
C	2.29583000	3.77010100	-0.24930700
C	3.87787100	4.24457100	1.98916400
H	2.19414600	5.29606900	2.77521300

C	3.60465000	3.27890100	-0.19507000
H	1.71616900	3.57316500	-1.14497200
C	4.40110500	3.50921400	0.92372900
H	4.48349200	4.43739400	2.87091100
H	3.99258400	2.71314800	-1.03582900
H	5.41490300	3.12062900	0.96733000
C	0.47214300	6.64721600	0.78521100
H	1.12879700	6.92013500	1.62112200
H	1.00734200	6.93231800	-0.12960000
C	-0.80073800	7.44523800	0.88833100
H	-1.37236100	7.33602700	1.81002700
C	-1.24928700	8.28483200	-0.04647100
H	-0.71586900	8.43623500	-0.98300400
H	-2.16637600	8.85231300	0.08582400

TS-EF-3SS

l imaginary frequency

H = -5236.781225

G = -5236.975533

E(M06-2X-DCM) = -5237.626868

E(M06-2X-cyclohexane) = -5237.599540

O	-0.64170300	-2.60455500	-0.68051100
O	-2.74045000	-1.07977100	-0.57933600
P	-1.12953700	-1.09465100	-0.27849800
O	-0.49557800	-0.04266900	-1.13948600
C	-1.05194600	-3.63497300	-4.72098000
C	-2.11367400	-3.78485600	-3.83490600
C	-1.94475200	-3.51047800	-2.47024800
C	0.36701000	-2.84780800	-2.88475000
C	0.18023300	-3.19991400	-4.23342600
C	-3.57948900	-1.98989700	0.07126100
C	-3.65639000	-3.30570200	-0.39103400
C	-4.36174200	-4.25660200	0.36443200
C	-5.07339500	-3.88132000	1.49780300
C	-5.09275600	-2.53751000	1.86592900
C	-4.34886500	-1.56662700	1.17444100
H	1.02415100	-3.10352500	-4.91012000
H	-5.68244900	-2.21918900	2.72055700
C	-3.17829000	-3.94770400	-1.69256600
C	-4.26726800	-3.82563000	-2.81285800
H	-4.59294700	-2.78072100	-2.87343000
H	-5.14982600	-4.43916100	-2.60670800
H	-5.13045600	-5.95988400	-0.73513100
H	-3.98205100	-6.39792700	0.52506400

C	-0.73554800	-2.98778800	-2.02048500
H	-1.17258700	-3.85681400	-5.77840200
H	-5.62104800	-4.61694600	2.08140100
C	-3.53610000	-4.21819400	-4.11573700
H	-3.95811600	-3.72872100	-5.00095700
H	-3.59436700	-5.30069900	-4.29707100
C	-4.20752700	-5.63839600	-0.23221700
C	-3.05580100	-5.44097400	-1.23953000
H	-2.09333900	-5.57581600	-0.73291800
H	-3.08979500	-6.13689400	-2.08357100
C	-4.49391900	-0.13971800	1.61098500
C	-4.00163100	0.27387600	2.87286700
C	-5.26594200	0.75165100	0.82331200
C	-3.20669000	-0.57633500	3.70583300
C	-4.29486100	1.60510700	3.35720500
C	-5.55335700	2.07961400	1.32003900
C	-2.74476700	-0.15118000	4.92315200
H	-2.93889300	-1.55879700	3.34143100
C	-3.80181800	2.00593900	4.63903200
C	-5.06281600	2.46887400	2.57070300
C	-3.05166200	1.15354300	5.40320000
H	-2.11763700	-0.80879300	5.51717400
H	-4.04050900	3.00661600	4.99258400
H	-5.30172600	3.46139800	2.94951700
H	-2.67983600	1.47047000	6.37394000
C	1.71254500	-2.37462200	-2.43611900
C	2.25609900	-1.18397300	-2.98094800
C	2.47647400	-3.15778500	-1.53543700
C	1.51478300	-0.31421000	-3.84647900
C	3.61027500	-0.79931800	-2.65076900
C	3.80846300	-2.73101000	-1.17184900
C	2.08022000	0.81521100	-4.37990500
H	0.48142000	-0.55505900	-4.06495000
C	4.16855400	0.38044000	-3.23957400
C	4.34512000	-1.57867300	-1.75304300
C	3.42969700	1.16419200	-4.08502000
H	1.49333900	1.45451900	-5.03462400
H	5.19336600	0.64605400	-2.99113100
H	5.35955700	-1.27962700	-1.49784300
H	3.86571700	2.05522500	-4.52943900
C	-6.57552000	1.26673600	-1.17815300
H	-6.97702000	0.96212500	-2.14065600
C	-5.81731200	0.38889900	-0.44786400
H	-5.62906300	-0.60596700	-0.83419100

C	-6.84947200	2.57462600	-0.68694200
H	-7.45974600	3.25478400	-1.27502900
C	-6.35426200	2.96348300	0.52930500
H	-6.57248600	3.95274400	0.92646400
C	2.75611100	-5.10281600	-0.08296800
H	2.36443900	-6.02652000	0.33457100
C	4.05032500	-4.65340000	0.30354100
H	4.62857100	-5.22829100	1.02166500
C	4.56154300	-3.50322600	-0.23283800
H	5.54386800	-3.14343400	0.06016200
C	1.99953100	-4.38344100	-0.97012700
H	1.01843200	-4.74588800	-1.25358100
C	-1.62290300	3.79518500	-0.59110800
C	-1.68073700	3.95667400	0.97435800
H	-1.39595100	4.98099000	1.23918500
H	-2.72871800	3.82401200	1.28158900
C	-0.87690200	2.99879600	1.78091100
C	-0.15223700	3.61440900	-1.03351900
H	0.42813800	4.50180400	-0.78397600
H	-0.12378800	3.47952000	-2.12022800
N	0.54801000	2.46082500	-0.44417100
C	1.80154300	2.51352900	0.04469200
N	2.50684200	1.36748800	0.11676400
C	3.88280600	1.26359100	0.47154400
C	4.83005500	2.02888200	-0.20991300
C	4.28935600	0.33271900	1.43271200
C	6.18513600	1.87721900	0.08216400
C	5.64862500	0.19312200	1.71236400
H	3.54845400	-0.27834900	1.93332600
C	6.60406000	0.96370900	1.04711500
H	7.65756500	0.85201900	1.27567300
C	6.11863800	-0.83735700	2.70651400
C	7.19081400	2.63899100	-0.73818200
F	7.10528500	-0.34907300	3.49187600
F	6.63270400	-1.92620000	2.07866100
F	5.12905300	-1.26722500	3.50818000
F	7.38056400	2.04745200	-1.94646800
F	8.39565000	2.70418300	-0.13731600
F	6.78402900	3.90197200	-0.98625300
S	2.39670800	3.98173800	0.77079900
H	4.51539000	2.71889000	-0.98342500
H	2.01048800	0.47665600	0.01146100
H	0.20445300	1.52800900	-0.75002600
C	0.07845500	3.41996600	2.69077300

H	0.00243400	4.43929400	3.07701100
H	1.10484400	3.71933000	1.85164400
H	0.50437300	2.67573600	3.36138200
N	-1.01299700	-0.99189900	1.33140000
S	0.36196200	-0.98728900	2.11432100
O	0.38630000	0.03967700	3.16753700
O	1.56243400	-1.08594700	1.24187400
C	0.35526900	-2.61527300	3.03141700
F	0.26786400	-3.63156200	2.17120900
F	-0.68452900	-2.67547100	3.87838900
F	1.48552400	-2.73046100	3.73569200
H	-1.03850800	1.93013400	1.65603100
C	-2.19468900	5.09345700	-1.20096300
C	-3.49624400	5.49793400	-0.85540000
C	-1.48020200	5.91265200	-2.08703500
C	-4.05523100	6.66814000	-1.36451200
H	-4.09404800	4.88802100	-0.18436100
C	-2.03850000	7.08592600	-2.60211600
H	-0.47610200	5.65120000	-2.40063100
C	-3.32695000	7.47239900	-2.24282500
H	-5.06417000	6.94985500	-1.07448700
H	-1.45628500	7.69501200	-3.28851900
H	-3.76031100	8.38522700	-2.64211900
C	-2.50679500	2.58351100	-1.03638300
H	-3.54416100	2.80921100	-0.77557700
H	-2.22626100	1.70000800	-0.45615500
C	-2.41870000	2.24104700	-2.50302000
H	-1.57433800	1.62125300	-2.79972300
C	-3.31011600	2.61487600	-3.42232700
H	-3.20413200	2.33135200	-4.46655600
H	-4.18406700	3.20953100	-3.16621400

TS-EF-3SS-1

l imaginary frequency

H = -5236.781225

G = -5236.975534

E(M06-2X-DCM) = -5237.626868

E(M06-2X-cyclohexane) = -5237.599541

O	-0.64169400	-2.60456500	-0.68051100
O	-2.74043100	-1.07976800	-0.57933800
P	-1.12951800	-1.09465800	-0.27849800
O	-0.49555000	-0.04268300	-1.13949000
C	-1.05191900	-3.63496600	-4.72098600
C	-2.11365500	-3.78484200	-3.83491900

C	-1.94473800	-3.51047100	-2.47026000
C	0.36703300	-2.84782100	-2.88474400
C	0.18026100	-3.19992100	-4.23342200
C	-3.57947700	-1.98989200	0.07125100
C	-3.65638500	-3.30569500	-0.39105300
C	-4.36174600	-4.25659600	0.36440400
C	-5.07340000	-3.88131700	1.49777600
C	-5.09275300	-2.53751000	1.86591200
C	-4.34885400	-1.56662700	1.17443300
H	1.02418400	-3.10353700	-4.91011100
H	-5.68244600	-2.21919200	2.72054000
C	-3.17828400	-3.94769200	-1.69258700
C	-4.26725500	-3.82560300	-2.81288400
H	-4.59292600	-2.78069100	-2.87345100
H	-5.14981900	-4.43912800	-2.60674200
H	-5.13046800	-5.95986300	-0.73517400
H	-3.98207200	-6.39792400	0.52502300
C	-0.73553200	-2.98779300	-2.02048600
H	-1.17255500	-3.85680200	-5.77841000
H	-5.62106000	-4.61694300	2.08136600
C	-3.53608300	-4.21816500	-4.11576100
H	-3.95808900	-3.72868300	-5.00098100
H	-3.59435900	-5.30066900	-4.29710200
C	-4.20753900	-5.63838600	-0.23225400
C	-3.05580700	-5.44096500	-1.23956000
H	-2.09334900	-5.57581800	-0.73294500
H	-3.08980300	-6.13688000	-2.08360700
C	-4.49390200	-0.13972000	1.61099000
C	-4.00161200	0.27385800	2.87287600
C	-5.26592400	0.75165800	0.82332700
C	-3.20667400	-0.57636400	3.70583300
C	-4.29484000	1.60508400	3.35722900
C	-5.55333800	2.07961500	1.32007000
C	-2.74475100	-0.15122400	4.92315700
H	-2.93887900	-1.55882200	3.34142100
C	-3.80179700	2.00590200	4.63906200
C	-5.06279500	2.46886100	2.57073700
C	-3.05164200	1.15349500	5.40322000
H	-2.11762300	-0.80884400	5.51717200
H	-4.04048500	3.00657500	4.99262400
H	-5.30170400	3.46138100	2.94956300
H	-2.67981600	1.47041000	6.37396400
C	1.71256900	-2.37464800	-2.43610300
C	2.25613800	-1.18400600	-2.98093200

C	2. 47648400	-3. 15781600	-1. 53541400
C	1. 51483800	-0. 31423600	-3. 84646900
C	3. 61031700	-0. 79936500	-2. 65074600
C	3. 80847400	-2. 73105300	-1. 17181700
C	2. 08029000	0. 81517700	-4. 37989500
H	0. 48147200	-0. 55507300	-4. 06494300
C	4. 16861300	0. 38038400	-3. 23955300
C	4. 34514700	-1. 57872300	-1. 75301000
C	3. 42977000	1. 16414100	-4. 08500600
H	1. 49341900	1. 45449000	-5. 03461800
H	5. 19342700	0. 64598700	-2. 99110700
H	5. 35958500	-1. 27968700	-1. 49780400
H	3. 86580300	2. 05516700	-4. 52942700
C	-6. 57550700	1. 26676600	-1. 17812800
H	-6. 97700800	0. 96216600	-2. 14063400
C	-5. 81729600	0. 38892000	-0. 44785200
H	-5. 62904800	-0. 60594100	-0. 83419000
C	-6. 84945800	2. 57465000	-0. 68690100
H	-7. 45973300	3. 25481500	-1. 27497900
C	-6. 35424500	2. 96349300	0. 52934800
H	-6. 57246900	3. 95274900	0. 92652000
C	2. 75609200	-5. 10284700	-0. 08293800
H	2. 36440900	-6. 02654600	0. 33460000
C	4. 05030700	-4. 65344200	0. 30358000
H	4. 62854300	-5. 22833600	1. 02170900
C	4. 56153900	-3. 50327400	-0. 23279800
H	5. 54386600	-3. 14348900	0. 06020700
C	1. 99952500	-4. 38346700	-0. 97010500
H	1. 01842600	-4. 74590600	-1. 25356600
C	-1. 62293500	3. 79517700	-0. 59112700
C	-1. 68077500	3. 95666500	0. 97433700
H	-1. 39599100	4. 98098100	1. 23916700
H	-2. 72875700	3. 82400300	1. 28156500
C	-0. 87694100	2. 99878700	1. 78089100
C	-0. 15226800	3. 61441600	-1. 03353200
H	0. 42810100	4. 50181200	-0. 78397700
H	-0. 12381100	3. 47953800	-2. 12024100
N	0. 54798400	2. 46083200	-0. 44418900
C	1. 80151500	2. 51354000	0. 04467600
N	2. 50682400	1. 36750500	0. 11673200
C	3. 88278800	1. 26361800	0. 47152300
C	4. 83003500	2. 02890700	-0. 20994100
C	4. 28933800	0. 33276800	1. 43271100
C	6. 18511500	1. 87726100	0. 08214800

C	5.64860800	0.19318800	1.71237500
H	3.54843600	-0.27829500	1.93333100
C	6.60404000	0.96377100	1.04711900
H	7.65754400	0.85209500	1.27568700
C	6.11861400	-0.83727400	2.70654600
C	7.19079400	2.63902600	-0.73820200
F	7.10533300	-0.34901400	3.49183200
F	6.63257600	-1.92617900	2.07871700
F	5.12904500	-1.26704200	3.50828600
F	7.38059300	2.04744300	-1.94645900
F	8.39561200	2.70427200	-0.13730700
F	6.78398400	3.90198600	-0.98633500
S	2.39667000	3.98174300	0.77080500
H	4.51536800	2.71890000	-0.98346500
H	2.01048300	0.47667200	0.01138300
H	0.20443300	1.52801300	-0.75004200
C	0.07840700	3.41995700	2.69076200
H	0.00238100	4.43928500	3.07700100
H	1.10480200	3.71932900	1.85163700
H	0.50432600	2.67572700	3.36136900
N	-1.01298100	-0.99190400	1.33139900
S	0.36197700	-0.98729800	2.11432600
O	0.38630800	0.03966200	3.16754700
O	1.56245100	-1.08595300	1.24188400
C	0.35527700	-2.61528800	3.03141400
F	0.26787400	-3.63157200	2.17120100
F	-0.68452500	-2.67549000	3.87838200
F	1.48552800	-2.73048100	3.73569300
H	-1.03853800	1.93012500	1.65600300
C	-2.19473200	5.09344500	-1.20098400
C	-3.49629900	5.49789900	-0.85543800
C	-1.48024200	5.91265900	-2.08703600
C	-4.05529600	6.66810100	-1.36454900
H	-4.09410500	4.88797000	-0.18441500
C	-2.03855000	7.08592900	-2.60211500
H	-0.47613300	5.65122600	-2.40061700
C	-3.32701300	7.47237900	-2.24284300
H	-5.06424300	6.94979800	-1.07453800
H	-1.45633300	7.69503100	-3.28850300
H	-3.76038000	8.38520400	-2.64213500
C	-2.50681300	2.58349400	-1.03640800
H	-3.54418500	2.80919000	-0.77562400
H	-2.22628600	1.69999900	-0.45616600
C	-2.41868700	2.24101700	-2.50304000

H	-1.57433500	1.62119500	-2.79971300
C	-3.31006500	2.61486900	-3.42237600
H	-3.20405800	2.33133500	-4.46660000
H	-4.18400200	3.20955500	-3.16629300

TS-EF-3SS-2

1 imaginary frequency

H = -5236.776152

G = -5236.971133

E(M06-2X-DCM) = -5237.618648

E(M06-2X-cyclohexane) = -5237.590276

O	-1.17350400	-2.61418100	-0.26415900
O	-2.82801700	-0.72772000	0.39365000
P	-1.24503100	-1.01293100	0.07381300
O	-0.90258700	-0.15610500	-1.11003600
C	-3.20187600	-3.87434800	-3.69880300
C	-3.87069200	-3.74093600	-2.48594800
C	-3.16995800	-3.39616000	-1.32089300
C	-1.10466400	-3.22147200	-2.61554600
C	-1.82580700	-3.64538000	-3.74505200
C	-3.47448500	-1.42051100	1.41862900
C	-3.93650400	-2.71704100	1.18568300
C	-4.44789600	-3.45972300	2.26285500
C	-4.60076400	-2.88352000	3.51892400
C	-4.23956900	-1.54894400	3.70001900
C	-3.66003300	-0.79362300	2.66804500
H	-1.29001500	-3.76902700	-4.68175400
H	-4.38344400	-1.07521300	4.66673000
C	-4.08166400	-3.52556800	-0.10506100
C	-5.47309600	-3.27642600	-0.78095700
H	-5.63149000	-2.19546600	-0.87273000
H	-6.30210600	-3.68568300	-0.19523500
H	-5.83535600	-5.04133800	1.73468000
H	-4.39218300	-5.61915800	2.56087100
C	-1.81694900	-3.07967100	-1.40832800
H	-3.73786500	-4.15537800	-4.60195700
H	-5.00141900	-3.45897400	4.34961800
C	-5.34525400	-3.90546400	-2.18662100
H	-5.98252800	-3.41246300	-2.92970600
H	-5.63500000	-4.96558900	-2.17816400
C	-4.75309200	-4.87922200	1.83747100
C	-4.03627600	-4.97950800	0.47482800
H	-2.98871800	-5.26283200	0.62793200
H	-4.48571900	-5.71296300	-0.20184200

C	-3.31132000	0.64047700	2.92755600
C	-2.26581200	0.97003300	3.82444000
C	-4.09949800	1.66606900	2.34788900
C	-1.43901900	-0.01909600	4.44609800
C	-1.99510700	2.35796500	4.12955600
C	-3.80512900	3.05046200	2.64548200
C	-0.44052800	0.33138400	5.31507900
H	-1.58713100	-1.05965500	4.18936900
C	-0.94770000	2.68034400	5.04878200
C	-2.76105100	3.35803700	3.52300600
C	-0.19445300	1.69738200	5.63039700
H	0.18982000	-0.43999900	5.74666400
H	-0.76483100	3.72868200	5.27419800
H	-2.55532300	4.40085700	3.75870600
H	0.60266400	1.95403800	6.32276000
C	0.36231300	-2.94469300	-2.72250300
C	0.82385800	-1.89226000	-3.55283800
C	1.29077000	-3.76213200	-2.03141900
C	-0.05804400	-1.01852200	-4.26863000
C	2.24495300	-1.66307700	-3.69324300
C	2.70610900	-3.49357400	-2.14684700
C	0.42278900	-0.03326600	-5.09330000
H	-1.12712900	-1.14355600	-4.14721900
C	2.70490200	-0.62002100	-4.55808400
C	3.14512100	-2.46117000	-2.98049000
C	1.82461900	0.16889500	-5.24837000
H	-0.27333200	0.59989300	-5.63827400
H	3.77783600	-0.47271700	-4.65874100
H	4.21369300	-2.27922200	-3.07961300
H	2.18884400	0.94982800	-5.91075200
C	-5.97467000	2.41030200	0.96422400
H	-6.82591200	2.17446400	0.33170300
C	-5.21999700	1.39780600	1.49708700
H	-5.47833600	0.36637400	1.28549100
C	-5.66044200	3.77251800	1.23514600
H	-6.26972700	4.56244100	0.80397200
C	-4.60622900	4.07854500	2.05444500
H	-4.37020400	5.11383900	2.29189300
C	1.81717600	-5.63243600	-0.55074200
H	1.48640200	-6.46885100	0.05911900
C	3.20674200	-5.33485700	-0.63530500
H	3.92111000	-5.93618700	-0.07980100
C	3.63645100	-4.29691100	-1.41609800
H	4.69310800	-4.05125900	-1.48312500

C	0.89476400	-4.87426100	-1.22240500
H	-0.15858800	-5.11802700	-1.14541600
C	-1.48653500	3.29855300	-2.16774600
C	-1.76174800	3.06124500	-0.65724600
H	-2.72986400	3.50041100	-0.37358300
H	-1.89585200	1.98853300	-0.50326000
C	-0.74271000	3.54270500	0.31759100
C	0.01171500	2.92861800	-2.47516000
H	0.61275700	3.82754000	-2.59425000
H	0.05963500	2.36667300	-3.41498600
N	0.66416400	2.10179600	-1.45248200
C	1.93511300	2.28623700	-1.03315300
N	2.57273100	1.21207300	-0.53942300
C	3.88593100	1.11068800	0.00173500
C	4.39965300	1.98373000	0.96230300
C	4.64151400	0.01631700	-0.42445000
C	5.68867400	1.77512900	1.45335000
C	5.92134500	-0.18921800	0.08689100
H	4.21895800	-0.67368500	-1.14576500
C	6.45851000	0.69379400	1.02196800
H	7.45541200	0.53821600	1.41628600
C	6.69410200	-1.40506300	-0.35316000
C	6.27584600	2.75889400	2.43215900
F	6.30410400	-2.51675600	0.30837000
F	8.02016900	-1.26280200	-0.15019300
F	6.51135700	-1.65945800	-1.67399100
F	6.95266200	3.74383800	1.79634100
F	7.14802300	2.16546300	3.27545800
F	5.32358000	3.35535200	3.18023500
S	2.63363800	3.87426100	-1.05168500
H	3.80309500	2.80443300	1.33420000
H	2.08834000	0.30304500	-0.54845600
H	0.23517100	1.16507400	-1.31892800
C	-0.00241900	4.72334500	0.27335400
H	-0.32988500	5.51408000	-0.40155400
H	1.12330100	4.38766000	-0.31417900
H	0.41936400	5.06585000	1.21952000
N	-0.47913500	-0.82606200	1.48065800
S	1.08221800	-1.04729100	1.66211600
O	1.67279600	-0.05377000	2.56465700
O	1.80032900	-1.31662900	0.38468900
C	1.20123100	-2.66544200	2.59139100
F	0.60094600	-2.55621500	3.78759100
F	2.48747600	-2.97154800	2.78660500

F	0.61550300	-3.65119100	1.90821700
C	-1.77057800	4.72986000	-2.66059900
C	-1.27741600	5.13720200	-3.91356900
C	-2.56411400	5.64568700	-1.95326800
C	-1.54680400	6.40456000	-4.42765900
H	-0.67400200	4.45480600	-4.50612300
C	-2.83640100	6.91760400	-2.46484500
H	-2.98509800	5.37992800	-0.98904400
C	-2.32792600	7.30561700	-3.70273200
H	-1.14495300	6.68610000	-5.39730900
H	-3.45095400	7.60349200	-1.88766000
H	-2.53870700	8.29477000	-4.09939000
C	-2.39456400	2.30341900	-2.97668400
H	-2.14139100	2.43507200	-4.03875700
H	-2.11060600	1.28324000	-2.69645100
C	-3.87629400	2.48568600	-2.80457600
C	-4.68682600	1.55982300	-2.28867800
H	-4.30769900	0.60732800	-1.92518100
H	-5.75747300	1.72524000	-2.20382800
H	-4.29410100	3.43225000	-3.14780400
H	-0.57534800	2.88546800	1.17141000

TS-EF-3SS-3

l imaginary frequency

H = -5236.774664

G = -5236.970648

E(M06-2X-DCM) = -5237.619682

E(M06-2X-cyclohexane) = -5237.591132

O	1.07380000	-2.44144600	0.94970200
O	2.99128100	-0.80546700	0.34201900
P	1.36268200	-0.97004200	0.28908200
O	0.76058600	0.14985300	1.08003000
C	2.14589400	-2.88356200	4.97168800
C	3.07636900	-3.09171300	3.95836800
C	2.69043100	-3.01500700	2.61267900
C	0.42007600	-2.43236900	3.29317300
C	0.82583100	-2.58632100	4.63024200
C	3.80177200	-1.73694800	-0.31464100
C	4.05546300	-2.97305700	0.28336200
C	4.71760400	-3.96584200	-0.45758400
C	5.21670500	-3.69558500	-1.72657500
C	5.07108800	-2.41119100	-2.24926400
C	4.36255100	-1.40969900	-1.56626900
H	0.08536900	-2.44446800	5.41214900

H	5. 50022600	-2. 16799100	-3. 21697000
C	3. 82916900	-3. 47123700	1. 71089700
C	5. 05509100	-3. 13496200	2. 62781300
H	5. 30018200	-2. 07299000	2. 51083100
H	5. 94556200	-3. 71429300	2. 36451700
H	5. 78097300	-5. 45847500	0. 70152400
H	4. 49988200	-6. 13038400	-0. 30154100
C	1. 39214400	-2. 62937300	2. 29376500
H	2. 43590900	-2. 95254400	6. 01717900
H	5. 72894100	-4. 46474000	-2. 29905200
C	4. 55477900	-3. 39713400	4. 06616300
H	5. 06092000	-2. 77123400	4. 81002500
H	4. 72502900	-4. 44108100	4. 36504000
C	4. 77013300	-5. 26571600	0. 31531200
C	3. 76731700	-5. 01518100	1. 46106300
H	2. 75540400	-5. 27671600	1. 13124200
H	3. 98435400	-5. 59286000	2. 36507300
C	4. 32660400	-0. 03298500	-2. 15965200
C	3. 57319900	0. 23341500	-3. 32771600
C	5. 17198700	0. 96720100	-1. 61532800
C	2. 72496900	-0. 74403900	-3. 93956800
C	3. 64661400	1. 53993800	-3. 94509700
C	5. 24268200	2. 26611400	-2. 24751300
C	2. 00894000	-0. 45731400	-5. 07130700
H	2. 62879000	-1. 71509100	-3. 47258500
C	2. 88444400	1. 79692200	-5. 12830800
C	4. 47122800	2. 51979800	-3. 38594200
C	2. 09086100	0. 82774300	-5. 67942700
H	1. 35299000	-1. 21098100	-5. 49572700
H	2. 95744600	2. 78226300	-5. 58345600
H	4. 53625600	3. 49563500	-3. 86432900
H	1. 51665400	1. 03421900	-6. 57876700
C	-1. 00229300	-2. 08877400	2. 98453000
C	-1. 53674300	-0. 84718300	3. 41114800
C	-1. 82828700	-3. 02548300	2. 31568600
C	-0. 74461300	0. 16542600	4. 04507500
C	-2. 93600300	-0. 55717200	3. 18946000
C	-3. 21319100	-2. 70210700	2. 05853000
C	-1. 29900300	1. 34608800	4. 46969800
H	0. 31655200	-0. 00916800	4. 17430400
C	-3. 47586100	0. 68497600	3. 65212900
C	-3. 73247700	-1. 48770200	2. 51552700
C	-2. 68693100	1. 60983600	4. 28176100
H	-0. 67430500	2. 08919900	4. 95964500

H	-4.53450900	0.87608600	3.49141400
H	-4.78214800	-1.26058900	2.34078100
H	-3.11210500	2.54545200	4.63570200
C	6.84897400	1.71418600	0.00152300
H	7.47711400	1.50966900	0.86426000
C	6.01078700	0.74094100	-0.47637800
H	5.98516200	-0.22894600	0.00677700
C	6.90967000	2.99285100	-0.62171600
H	7.58494000	3.75093300	-0.23377100
C	6.12472100	3.25756900	-1.71208600
H	6.16774800	4.22675000	-2.20420500
C	-2.17554600	-5.17678600	1.21061700
H	-1.78895600	-6.13991900	0.88842200
C	-3.52707500	-4.83364900	0.92354200
H	-4.15508600	-5.52812500	0.37247100
C	-4.03050900	-3.63293600	1.34383800
H	-5.05827100	-3.35719100	1.12445500
C	-1.35855200	-4.30658900	1.88294800
H	-0.33354800	-4.58806600	2.09421700
C	0.96984700	4.03709200	0.71662900
C	1.08853600	4.10808900	-0.83798300
H	0.57074900	5.00013200	-1.20625700
H	2.15096800	4.22918700	-1.09725400
C	0.58031300	2.93239800	-1.60024600
C	-0.47292100	3.58569100	1.09178200
H	-1.17707600	4.37636300	0.83416800
H	-0.53059700	3.41749000	2.17148300
N	-0.96496300	2.33998600	0.46710200
C	-2.19496100	2.23008500	-0.08191700
N	-2.80756100	1.03002100	-0.05164100
C	-4.13142300	0.73410100	-0.47761700
C	-5.19797900	1.57700000	-0.14966900
C	-4.37658300	-0.47413000	-1.14022100
C	-6.49545800	1.23255700	-0.52796000
C	-5.68296300	-0.81391500	-1.48777500
H	-3.55198500	-1.13923900	-1.36422100
C	-6.74943500	0.03766600	-1.19980100
H	-7.76077800	-0.23024000	-1.48178900
C	-5.95794100	-2.15277700	-2.12305400
C	-7.62601800	2.18399000	-0.23350700
F	-6.98656900	-2.08640100	-2.99709500
F	-6.30336400	-3.07606700	-1.18874600
F	-4.88803400	-2.63507500	-2.78073200
F	-7.41031900	2.87723300	0.90737700

F	-8.80354100	1.53647300	-0.10007600
F	-7.78305500	3.09197800	-1.22201300
S	-2.83561300	3.56673600	-0.99336200
H	-5.02884800	2.48526800	0.41421400
H	-2.23171400	0.20393100	0.15145500
H	-0.50991000	1.47532600	0.81002200
C	-0.30837300	3.08085600	-2.65031500
H	-0.34824300	4.05041000	-3.15302700
H	-1.44367800	3.33547600	-1.93364700
H	-0.54823200	2.20669900	-3.25261000
N	1.00497300	-1.12496300	-1.28271700
S	-0.48648900	-1.24395300	-1.78650400
O	-0.80281600	-0.28780700	-2.85935700
O	-1.48865400	-1.37233400	-0.69030700
C	-0.55328000	-2.92174600	-2.60199400
F	-0.23870000	-3.87704300	-1.72615500
F	0.29987500	-2.98388700	-3.63545100
F	-1.79412200	-3.13293500	-3.05677100
H	0.90341200	1.93232400	-1.32116800
C	1.17352800	5.43529100	1.34206100
C	1.65698100	6.53522200	0.61936400
C	0.90275600	5.63313700	2.70793300
C	1.84300000	7.78017200	1.22487400
H	1.91081100	6.43815200	-0.43009400
C	1.08178900	6.87482200	3.31554500
H	0.55603300	4.80709300	3.32154400
C	1.55059800	7.96001000	2.57468600
H	2.22149400	8.60905000	0.63250100
H	0.85701700	6.99046800	4.37259600
H	1.69204200	8.92886900	3.04550600
C	2.02211100	3.05731800	1.33423500
H	1.85455400	2.04695400	0.94791500
H	1.82128900	2.99699000	2.41050200
C	3.46141000	3.44454600	1.12556700
H	3.86856700	3.31386600	0.12367400
C	4.27184000	3.89336200	2.08459300
H	5.31165300	4.13298400	1.88082700
H	3.92981600	4.03067400	3.10845600

TS-EF-3SS-4

l imaginary frequency

H = -5236.777551

G = -5236.975236

E(M06-2X-DCM) = -5237.619385

E(M06-2X-cyclohexane) = -5237.591832

O	-1.23244000	-2.56360300	-0.57899400
O	-3.06694700	-0.76075200	-0.22723500
P	-1.44497100	-0.97851100	-0.22855500
O	-0.87698400	-0.05962500	-1.26716400
C	-2.54348500	-3.77696200	-4.36333400
C	-3.42198200	-3.73412700	-3.28517400
C	-2.95965400	-3.40009900	-2.00427800
C	-0.71097100	-3.07514000	-2.89809400
C	-1.19638100	-3.47807700	-4.15411300
C	-3.87030700	-1.50264100	0.64264400
C	-4.19411200	-2.82314700	0.32762700
C	-4.84824100	-3.61107800	1.28894900
C	-5.27291400	-3.06086700	2.49317500
C	-5.06028200	-1.70256900	2.72795900
C	-4.35536200	-0.89728100	1.81938800
H	-0.49610400	-3.53455900	-4.98247900
H	-5.43201300	-1.24533100	3.64039500
C	-4.06077700	-3.61370400	-0.97385500
C	-5.32449300	-3.42221000	-1.88132500
H	-5.53031200	-2.34960500	-1.97478800
H	-6.21636500	-3.89803500	-1.46180400
H	-6.01691400	-5.26705400	0.51774900
H	-4.70471700	-5.76817100	1.57868200
C	-1.63313900	-3.01487600	-1.83650800
H	-2.89427100	-4.04376400	-5.35714100
H	-5.77973600	-3.67151400	3.23609700
C	-4.91275700	-3.99338000	-3.25672600
H	-5.43995000	-3.51241300	-4.08856000
H	-5.13111000	-5.06842300	-3.32526900
C	-4.98143700	-5.03981000	0.80791400
C	-4.03415100	-5.07376600	-0.41030900
H	-3.01466900	-5.30365800	-0.08019900
H	-4.31776900	-5.81646300	-1.16263300
C	-4.23596600	0.57081800	2.09801800
C	-3.41112200	1.04471200	3.14552700
C	-5.05854800	1.47306600	1.37659900
C	-2.57376300	0.17940900	3.91916200
C	-3.39204700	2.45687900	3.45967500
C	-5.03556900	2.88140900	1.70516100
C	-1.78180300	0.66670200	4.92464600
H	-2.54707900	-0.87396300	3.67462500
C	-2.55373500	2.92383800	4.52098600
C	-4.19823700	3.33491100	2.72975000

C	-1. 77286800	2. 05624900	5. 23580000
H	-1. 13557100	-0. 01091800	5. 47396600
H	-2. 55641500	3. 98748000	4. 74909800
H	-4. 19407900	4. 39412000	2. 98166000
H	-1. 13875800	2. 42286400	6. 03862200
C	0. 74249200	-2. 76258100	-2. 72956300
C	1. 31322700	-1. 65729400	-3. 40762000
C	1. 56030300	-3. 61713400	-1. 94959500
C	0. 53756600	-0. 73681200	-4. 18555600
C	2. 73663300	-1. 41920700	-3. 31566800
C	2. 97654800	-3. 34969700	-1. 84353700
C	1. 12514500	0. 30634100	-4. 85482600
H	-0. 53667500	-0. 86902200	-4. 22929200
C	3. 30964800	-0. 31937400	-4. 02997000
C	3. 52648100	-2. 26579600	-2. 53299300
C	2. 53287100	0. 51737000	-4. 78533600
H	0. 51154200	0. 98039500	-5. 44751700
H	4. 38545900	-0. 17033100	-3. 96629400
H	4. 59653300	-2. 07995200	-2. 46228200
H	2. 98302800	1. 34302400	-5. 33015600
C	-6. 76836800	1. 94171600	-0. 30950800
H	-7. 44478200	1. 58937200	-1. 08346800
C	-5. 95924900	1. 05012400	0. 34556300
H	-6. 00512300	-0. 00252600	0. 09123500
C	-6. 73732700	3. 32771700	0. 01588900
H	-7. 39123600	4. 01959700	-0. 50827400
C	-5. 89135700	3. 77979400	0. 99291500
H	-5. 86193800	4. 83472800	1. 25601700
C	1. 87020900	-5. 57138700	-0. 51536200
H	1. 45537200	-6. 43619200	-0. 00452900
C	3. 26073200	-5. 28979100	-0. 39766300
H	3. 89240000	-5. 93635600	0. 20528600
C	3. 79485100	-4. 21174000	-1. 04876200
H	4. 85665700	-3. 98881800	-0. 97569300
C	1. 05281000	-4. 76790200	-1. 26577500
H	-0. 00110300	-5. 00593100	-1. 35038700
C	-0. 87527200	3. 56748800	-1. 47094600
C	-1. 15111100	3. 08441000	-0. 01728700
H	-2. 02030800	3. 61787600	0. 39438700
H	-1. 45595200	2. 03778700	-0. 06693700
C	-0. 04720600	3. 19487800	0. 98131800
C	0. 49797900	2. 96229600	-1. 96191000
H	1. 24031600	3. 74840500	-2. 07931300
H	0. 35159900	2. 48072600	-2. 93447500

N	1. 09409300	1. 94622000	-1. 08641900
C	2. 37591500	1. 96526400	-0. 66421300
N	2. 90474800	0. 81087000	-0. 22468900
C	4. 19994800	0. 66027000	0. 35507900
C	4. 30833400	0. 25321600	1. 68651800
C	5. 34233600	0. 85389700	-0. 42259700
C	5. 57626200	0. 05041800	2. 23529900
C	6. 60177000	0. 65674700	0. 14233400
H	5. 24468400	1. 15739500	-1. 45860000
C	6. 72565500	0. 25331600	1. 47204100
H	7. 70590300	0. 10991100	1. 91050100
C	7. 82903700	0. 80987000	-0. 71742400
C	5. 70043300	-0. 43412100	3. 65805600
F	8. 10577300	-0. 33277800	-1. 38940300
F	8. 92174000	1. 11295600	0. 01398400
F	7. 67249000	1. 77979700	-1. 64420000
F	6. 87497300	-0. 05658000	4. 21150800
F	5. 64747600	-1. 78285100	3. 72632800
F	4. 70930300	0. 04329400	4. 43716900
S	3. 23664900	3. 46751100	-0. 54050100
H	3. 41291600	0. 11794600	2. 28438500
H	2. 28966400	-0. 01007400	-0. 10695600
H	0. 58009900	1. 04737000	-1. 09260100
C	0. 82303100	4. 26735800	1. 16425300
H	0. 56326500	5. 23005400	0. 72481700
H	1. 85166800	3. 97207700	0. 40559400
H	1. 33941300	4. 31426700	2. 12389400
N	-0. 98758000	-0. 81701800	1. 31642200
S	0. 50087200	-0. 99843600	1. 80412100
O	0. 93020500	0. 09238500	2. 69958000
O	1. 46704800	-1. 38061800	0. 73591300
C	0. 43307500	-2. 51553000	2. 89205200
F	-0. 40670800	-2. 31730200	3. 91957100
F	1. 65249200	-2. 76471300	3. 37867600
F	0. 01516000	-3. 56951700	2. 18965800
C	-0. 87171900	5. 09706400	-1. 65257200
C	-0. 31437100	5. 65499900	-2. 81676500
C	-1. 48372400	5. 97925100	-0. 75028200
C	-0. 34066500	7. 02841400	-3. 05514800
H	0. 14513600	5. 01073400	-3. 56153200
C	-1. 50974800	7. 35685900	-0. 98167700
H	-1. 95252900	5. 60359500	0. 15314200
C	-0. 93547600	7. 89059200	-2. 13352600
H	0. 10573900	7. 42280500	-3. 96415000

H	-1.98655500	8.01028900	-0.25573800
H	-0.95473800	8.96178500	-2.31369100
C	-2.00108500	2.97290900	-2.39831700
H	-1.77991100	3.29088900	-3.42463300
H	-1.90364500	1.88026800	-2.36133800
C	-3.40956700	3.36549000	-2.05046300
C	-4.16807800	4.18662900	-2.77837300
H	-3.80017900	4.64963700	-3.69205800
H	-5.18737200	4.42343100	-2.48645400
H	-3.83318600	2.91997800	-1.15151600
H	0.07453500	2.33563600	1.64330300

TS-EF-3SS-5

1 imaginary frequency

H = -5236.782225

G = -5236.975623

E(M06-2X-DCM) = -5237.623252

E(M06-2X-cyclohexane) = -5237.596963

O	-0.80291300	-2.61844000	-0.48184500
O	-2.89303000	-1.08674500	-0.61617300
P	-1.29212400	-1.07027400	-0.27169200
O	-0.64371600	-0.11005000	-1.22200100
C	-1.10458500	-4.09720000	-4.38960600
C	-2.19546700	-4.13628400	-3.52737200
C	-2.06606200	-3.71386600	-2.19637300
C	0.26978500	-3.13427200	-2.60442400
C	0.11947300	-3.62951000	-3.91201000
C	-3.75840700	-1.91113000	0.10707100
C	-3.84030100	-3.26782600	-0.20980100
C	-4.58225100	-4.12088200	0.62312200
C	-5.32231800	-3.61293700	1.68468600
C	-5.33063500	-2.23635800	1.90356700
C	-4.55031000	-1.35776600	1.13338200
H	0.98654900	-3.62252800	-4.56580100
H	-5.94028700	-1.81893900	2.69948800
C	-3.32994300	-4.05246100	-1.41660500
C	-4.38099800	-4.04335800	-2.57881500
H	-4.69097300	-3.00830500	-2.76392800
H	-5.27775800	-4.62190200	-2.33610100
H	-5.34016800	-5.92635900	-0.30823200
H	-4.23803000	-6.23593300	1.02897400
C	-0.86331700	-3.15684500	-1.76949500
H	-1.19611900	-4.43233800	-5.41975600
H	-5.89983500	-4.27247600	2.32744800

C	-3.61405300	-4.58347800	-3.80596700
H	-4.00107300	-4.18980300	-4.75283500
H	-3.68124200	-5.67865500	-3.87000200
C	-4.42900100	-5.56149200	0.18645300
C	-3.24329900	-5.48832400	-0.79868700
H	-2.29924900	-5.57741900	-0.24914300
H	-3.26110200	-6.27266100	-1.56178500
C	-4.66905200	0.11143800	1.40125700
C	-4.23176100	0.64737600	2.63739000
C	-5.34809900	0.93705600	0.46904600
C	-3.51135200	-0.12726700	3.60185000
C	-4.49965500	2.03306200	2.95392500
C	-5.59888700	2.32440700	0.79239600
C	-3.10258400	0.41621500	4.79083200
H	-3.25467200	-1.15026800	3.36110400
C	-4.06834600	2.55742700	4.21319300
C	-5.17548300	2.83159100	2.02581100
C	-3.39291000	1.77319900	5.10893100
H	-2.53035300	-0.18834200	5.48790200
H	-4.29031300	3.59768900	4.44126300
H	-5.39542800	3.86809200	2.27718900
H	-3.06621900	2.18423700	6.06042300
C	1.61397100	-2.65241700	-2.16021100
C	2.21590500	-1.54656900	-2.81126400
C	2.32358100	-3.35950600	-1.15736000
C	1.52805000	-0.74535300	-3.78043000
C	3.57740300	-1.18130100	-2.48980300
C	3.66261700	-2.94512200	-0.80500700
C	2.14965200	0.29917300	-4.41464900
H	0.48936700	-0.96627300	-3.99500300
C	4.19672400	-0.09575300	-3.18809800
C	4.25991900	-1.88636000	-1.49490100
C	3.50718500	0.62266500	-4.12796200
H	1.60095800	0.89146600	-5.14242500
H	5.22808500	0.15104600	-2.94743400
H	5.28047800	-1.60167800	-1.24808000
H	3.98786600	1.44407600	-4.65292400
C	-6.49852700	1.27485100	-1.66330000
H	-6.85480800	0.87893600	-2.61031400
C	-5.83818800	0.45365400	-0.78707300
H	-5.68345100	-0.58788200	-1.04289900
C	-6.72852500	2.64333200	-1.34554200
H	-7.25534900	3.27973200	-2.05131100
C	-6.29431600	3.14745000	-0.14909200

H	-6.47516100	4.18775600	0.11211400
C	2.49067400	-5.14119600	0.50736400
H	2.05245000	-5.99813700	1.01199900
C	3.79174300	-4.69966900	0.87946000
H	4.32907100	-5.21210000	1.67272800
C	4.36129200	-3.63599600	0.23425300
H	5.35024100	-3.28341900	0.51348100
C	1.78551600	-4.49747400	-0.47530000
H	0.79850300	-4.85384700	-0.74545600
C	-1.44903200	3.54844900	-0.89753400
C	-1.55094200	2.99617000	0.55598400
H	-2.49956200	3.31532100	1.01596200
H	-1.62747300	1.90663200	0.52288900
C	-0.48288700	3.34699100	1.52556300
C	0.00359600	3.29614400	-1.43133700
H	0.59887000	4.20400700	-1.38336600
H	-0.05307000	2.98626600	-2.48027400
N	0.76611600	2.26906600	-0.71176800
C	2.04133700	2.41773200	-0.29890100
N	2.68648400	1.29152400	0.07662400
C	4.04964500	1.15842600	0.43565900
C	4.38113100	0.31867400	1.50721200
C	5.06001300	1.76157000	-0.31556300
C	5.72146800	0.11059400	1.82620000
C	6.39667100	1.54211700	0.01854500
H	4.81098000	2.37213500	-1.17396400
C	6.73941200	0.72320100	1.09163100
H	7.77931500	0.56104100	1.34920400
C	7.46129800	2.12511900	-0.87145900
C	6.10048600	-0.82989800	2.94044800
F	7.56828700	1.41772700	-2.02665500
F	8.67692700	2.11651700	-0.28870500
F	7.18162800	3.39770500	-1.22310300
F	7.12234300	-0.33707900	3.67581900
F	6.52105400	-2.02557300	2.45293800
F	5.07524400	-1.07752000	3.77529700
S	2.74311200	3.99286600	-0.10697900
H	3.59399800	-0.17299700	2.06723300
H	2.11525800	0.45499000	0.25805700
H	0.40010100	1.30663500	-0.83761600
C	0.22860700	4.54781500	1.60239000
H	-0.18210900	5.41952300	1.09204600
H	1.26507200	4.33201900	0.89086500
H	0.71507500	4.75712500	2.55673000

N	-1.21351600	-0.79850400	1.32260900
S	0.12708800	-0.67308600	2.14473700
O	0.10086400	0.47271900	3.06982200
O	1.36999200	-0.85062900	1.34179700
C	0.11853900	-2.17918000	3.24948600
F	-0.95007300	-2.16049000	4.06028200
F	1.22460800	-2.18281900	3.99954300
F	0.08190900	-3.29052200	2.51309100
C	-1.82712800	5.04169900	-1.00880600
C	-1.19096400	5.90748400	-1.91482300
C	-2.90199900	5.56714900	-0.27022100
C	-1.58472800	7.24079400	-2.05017900
H	-0.38298600	5.54990200	-2.54393500
C	-3.29624400	6.89873500	-0.40009300
H	-3.45650700	4.93306200	0.41464100
C	-2.63492400	7.74780100	-1.28770700
H	-1.06480000	7.87983000	-2.75891500
H	-4.12595400	7.27060100	0.19554100
H	-2.93903700	8.78592600	-1.38814900
C	-2.48064500	2.71552900	-1.74753700
H	-2.22784600	1.65574500	-1.64866900
H	-3.47124500	2.86089200	-1.29772400
C	-2.54392300	3.07395700	-3.20687700
C	-2.18774700	2.24496600	-4.19174100
H	-1.81847900	1.24293500	-3.98239000
H	-2.26624600	2.53197500	-5.23756900
H	-2.91584200	4.06778100	-3.45481200
H	-0.23671700	2.55978400	2.24207300

TS-EF-3SS-6

l imaginary frequency

H = -5236.779668

G = -5236.973660

E(M06-2X-DCM) = -5237.621719

E(M06-2X-cyclohexane) = -5237.594507

O	-0.75086400	-2.63535400	-0.52040000
O	-2.86673000	-1.13438800	-0.59976000
P	-1.26300100	-1.10044300	-0.27201900
O	-0.63896600	-0.11085500	-1.20831500
C	-1.08593900	-4.03897100	-4.45268900
C	-2.16152300	-4.11835200	-3.57414500
C	-2.01931300	-3.71943900	-2.23729500
C	0.29735500	-3.08383100	-2.67039500
C	0.13576400	-3.55476600	-3.98552200

C	-3.71047200	-1.98554300	0.11820500
C	-3.77123800	-3.33856900	-0.21826700
C	-4.48627100	-4.21750500	0.61130400
C	-5.22187400	-3.73917200	1.68967800
C	-5.25526700	-2.36592800	1.92760700
C	-4.50223200	-1.46196000	1.16002500
H	0.99144200	-3.51579500	-4.65309400
H	-5.86395100	-1.97139100	2.73590900
C	-3.26439300	-4.09502000	-1.44448100
C	-4.33315100	-4.08630000	-2.59068100
H	-4.66588700	-3.05444800	-2.75259400
H	-5.21466000	-4.68661400	-2.34494300
H	-5.22358900	-6.02313500	-0.33620200
H	-4.09609700	-6.33146800	0.97993800
C	-0.82106200	-3.14750800	-1.81814300
H	-1.18748000	-4.35493200	-5.48793100
H	-5.77787200	-4.41895100	2.33032700
C	-3.57502400	-4.58921600	-3.83892800
H	-3.98472400	-4.18693200	-4.77251200
H	-3.62113400	-5.68427400	-3.92130000
C	-4.31221600	-5.64834100	0.15059000
C	-3.14270400	-5.53831200	-0.85056600
H	-2.18909800	-5.61867100	-0.31638000
H	-3.15791800	-6.31102100	-1.62552000
C	-4.65043200	0.00217100	1.44212900
C	-4.19176200	0.54384800	2.66750000
C	-5.37812800	0.81331800	0.53418800
C	-3.43420600	-0.21964300	3.61213800
C	-4.47765900	1.92380000	2.99387100
C	-5.65112800	2.19372500	0.86893800
C	-3.00416700	0.32966600	4.79082000
H	-3.16777000	-1.23834800	3.36391000
C	-4.02090000	2.45489400	4.24136300
C	-5.19738800	2.70936800	2.08801500
C	-3.30805400	1.68170800	5.11750800
H	-2.40453100	-0.26595600	5.47230500
H	-4.25514000	3.49077500	4.47690900
H	-5.43087600	3.74080000	2.34766700
H	-2.96299300	2.09758000	6.06037600
C	1.63890800	-2.58446300	-2.23723500
C	2.20607700	-1.44974500	-2.86949000
C	2.38108900	-3.30221100	-1.26606400
C	1.48364900	-0.63795700	-3.80425600
C	3.56595700	-1.06531800	-2.56368600

C	3. 71812900	-2. 87001500	-0. 92769900
C	2. 07309200	0. 43437700	-4. 42291600
H	0. 44503400	-0. 87277400	-4. 00370400
C	4. 15031600	0. 05039700	-3. 24443700
C	4. 28128000	-1. 78206400	-1. 60069400
C	3. 42922500	0. 77814800	-4. 15294100
H	1. 50061400	1. 03146600	-5. 12834500
H	5. 18110400	0. 31142800	-3. 01630400
H	5. 30071400	-1. 48353000	-1. 36586900
H	3. 88389700	1. 62168700	-4. 66588300
C	-6. 61801400	1. 12236600	-1. 55193900
H	-7. 00066800	0. 71790700	-2. 48493200
C	-5. 90017100	0. 31914500	-0. 70487400
H	-5. 72583700	-0. 71721300	-0. 96928100
C	-6. 87433400	2. 48341500	-1. 22119100
H	-7. 45221300	3. 10408500	-1. 90078200
C	-6. 40372200	2. 99917400	-0. 04322000
H	-6. 60238700	4. 03377100	0. 22732200
C	2. 61421400	-5. 12180200	0. 34888000
H	2. 20242400	-5. 99979400	0. 83937500
C	3. 91326700	-4. 66394500	0. 70817300
H	4. 47538400	-5. 18544500	1. 47799300
C	4. 44965500	-3. 57298000	0. 08035900
H	5. 43672400	-3. 20814700	0. 35039100
C	1. 87813300	-4. 46753700	-0. 60367400
H	0. 89313800	-4. 83617700	-0. 86457500
C	-1. 47051400	3. 51768100	-0. 86845200
C	-1. 56299100	2. 93151700	0. 57164000
H	-2. 51846000	3. 22149100	1. 03566900
H	-1. 61765700	1. 84190500	0. 51209900
C	-0. 50225700	3. 28258900	1. 55201100
C	-0. 01469800	3. 27666300	-1. 40910400
H	0. 57178200	4. 19047500	-1. 36466400
H	-0. 05727100	2. 96120400	-2. 45642800
N	0. 76055000	2. 25585300	-0. 69430400
C	2. 03202900	2. 41761200	-0. 27768200
N	2. 69447300	1. 29821500	0. 08484700
C	4. 06146600	1. 17985000	0. 43399300
C	4. 41210100	0. 32255900	1. 48544800
C	5. 05781200	1. 81351000	-0. 31060300
C	5. 75738600	0. 12696900	1. 79076600
C	6. 39977700	1. 60628400	0. 00985000
H	4. 79454900	2. 43764200	-1. 15497200
C	6. 76152000	0. 76960000	1. 06265000

H	7. 80535200	0. 61628100	1. 30931300
C	7. 44833100	2. 22552000	-0. 87485400
C	6. 15668200	-0. 83413500	2. 88023600
F	7. 53888100	1. 56089100	-2. 05641400
F	8. 67287200	2. 20145400	-0. 31199000
F	7. 15787800	3. 50875800	-1. 17572600
F	5. 14401200	-1. 10414000	3. 72346400
F	7. 18586200	-0. 35095300	3. 61162100
F	6. 57605700	-2. 01714200	2. 36227400
S	2. 70531800	4. 00332700	-0. 06018100
H	3. 63590600	-0. 19252700	2. 03970500
H	2. 13715900	0. 44923600	0. 25369700
H	0. 40264400	1. 29011600	-0. 82298600
C	0. 19014000	4. 48962700	1. 65229400
H	-0. 22584700	5. 36535400	1. 15371800
H	1. 24063500	4. 29968000	0. 92546200
H	0. 68224800	4. 68665200	2. 60611800
N	-1. 16786700	-0. 86078900	1. 32630600
S	0. 18204600	-0. 73254600	2. 13211700
O	0. 15832600	0. 39972500	3. 07366600
O	1. 41614700	-0. 88652800	1. 31022800
C	0. 20187400	-2. 25397200	3. 21513200
F	-0. 85532300	-2. 25499200	4. 04105500
F	1. 31850100	-2. 25914300	3. 94941200
F	0. 16354200	-3. 35522100	2. 46384200
C	-1. 84838600	5. 01270200	-0. 93811000
C	-1. 22666100	5. 89817300	-1. 83366100
C	-2. 91006400	5. 52121600	-0. 17047600
C	-1. 61819400	7. 23496200	-1. 93005400
H	-0. 43016600	5. 55500700	-2. 48543700
C	-3. 30477100	6. 85590600	-0. 26295500
H	-3. 45485900	4. 87245600	0. 50847800
C	-2. 65534500	7. 72518700	-1. 13937300
H	-1. 10866700	7. 88980400	-2. 63189500
H	-4. 12479400	7. 21431600	0. 35402800
H	-2. 95894800	8. 76594700	-1. 21007300
C	-2. 50967500	2. 70805800	-1. 73079200
H	-2. 20683900	1. 65344800	-1. 70409300
H	-3. 48614400	2. 77760000	-1. 23955100
C	-2. 65114400	3. 14601400	-3. 16337800
C	-3. 77927800	3. 60222000	-3. 70892700
H	-4. 69083500	3. 70846200	-3. 12524300
H	-3. 83575100	3. 87685200	-4. 75912800
H	-1. 77088100	3. 04545800	-3. 80029600

H -0.24658700 2.48692900 2.25561500

TS-EF-3SR

1 imaginary frequency

H = -5236.772475

G = -5236.968577

E(M06-2X-DCM) = -5237.621849

E(M06-2X-cyclohexane) = -5237.593322

O	-1.02715900	-2.38403900	-0.45169900
O	-2.89637700	-0.61143900	-0.16113500
P	-1.26590400	-0.80482600	-0.07150200
O	-0.63329800	0.13477300	-1.04769400
C	-2.06831100	-3.47296400	-4.35516800
C	-3.01911400	-3.46759700	-3.33921400
C	-2.64696000	-3.17805600	-2.01895900
C	-0.34338500	-2.82728000	-2.74134500
C	-0.73917500	-3.18484000	-4.04167600
C	-3.73757200	-1.39169100	0.63438100
C	-4.03407500	-2.70025800	0.24735300
C	-4.73923500	-3.53191600	1.13289800
C	-5.23846600	-3.03728100	2.33229900
C	-5.04763500	-1.69014700	2.63754700
C	-4.29648500	-0.84254700	1.80786900
H	0.01782800	-3.21586300	-4.82001700
H	-5.47413200	-1.27464400	3.54601300
C	-3.81243000	-3.43605300	-1.07395900
C	-5.01417400	-3.21584400	-2.05540900
H	-5.22085900	-2.14115300	-2.12121900
H	-5.92906400	-3.71104800	-1.71523500
H	-5.84762600	-5.15692900	0.21987500
H	-4.60289700	-5.69885200	1.34057900
C	-1.33703500	-2.79685300	-1.74468600
H	-2.34851500	-3.70570100	-5.37956400
H	-5.78406400	-3.68184700	3.01680900
C	-4.50733200	-3.73193900	-3.42108600
H	-4.98076800	-3.22168900	-4.26792700
H	-4.71511200	-4.80408300	-3.54510500
C	-4.83393200	-4.93929100	0.58502800
C	-3.81115600	-4.91831600	-0.57019500
H	-2.81311800	-5.15619200	-0.18496600
H	-4.04017400	-5.63090300	-1.36886900
C	-4.20513300	0.61070500	2.16328600
C	-3.44933900	1.03856300	3.28049200
C	-4.98689400	1.54380700	1.43606500

C	-2.66226800	0.13994600	4.06866100
C	-3.45366400	2.43577000	3.65586300
C	-4.96458400	2.94163600	1.80728200
C	-1.94664300	0.58159700	5.14942900
H	-2.61037100	-0.90015600	3.77623000
C	-2.69736500	2.85423400	4.79573400
C	-4.19622900	3.34890800	2.90238600
C	-1.96789800	1.95495900	5.52531400
H	-1.33565800	-0.11893600	5.71000900
H	-2.71954800	3.90657100	5.07030400
H	-4.19526600	4.39924200	3.18849900
H	-1.39523500	2.28452000	6.38813800
C	1.09507800	-2.53337900	-2.45746200
C	1.72405900	-1.41902400	-3.06546300
C	1.84353200	-3.40957800	-1.63270100
C	1.01173000	-0.46148400	-3.85987000
C	3.14153700	-1.20449900	-2.87204100
C	3.24681800	-3.15150900	-1.40420000
C	1.65772900	0.58941700	-4.45931800
H	-0.06165300	-0.56347000	-3.96398200
C	3.77793900	-0.10070000	-3.52457500
C	3.86043600	-2.06951000	-2.04172200
C	3.06288900	0.76842800	-4.30399300
H	1.08931900	1.29683600	-5.05744500
H	4.84808700	0.03181100	-3.38298900
H	4.92364200	-1.89729600	-1.88775700
H	3.56021900	1.59844000	-4.79941800
C	-6.60358800	2.08552900	-0.31999800
H	-7.25603900	1.76344400	-1.12729100
C	-5.84961800	1.16169800	0.35739400
H	-5.91382000	0.11319300	0.08834700
C	-6.54851400	3.46521500	0.02700100
H	-7.14868400	4.18408700	-0.52410200
C	-5.75294800	3.87555700	1.06278300
H	-5.71603500	4.92353800	1.35182000
C	2.02281300	-5.37998400	-0.19914600
H	1.56344600	-6.24984700	0.26263700
C	3.39428100	-5.09542600	0.05456400
H	3.96495000	-5.74020600	0.71720600
C	3.98810700	-4.01447800	-0.53772900
H	5.03061600	-3.77836000	-0.34359300
C	1.27667500	-4.56851600	-1.01256400
H	0.23467900	-4.80422000	-1.19432100
C	-0.98017500	4.02709500	-1.56748900

C	-1.35553100	4.14272500	-0.05290900
H	-1.05027800	5.13655100	0.29425300
H	-2.44880900	4.11770300	0.04642400
C	-0.77682000	3.12318300	0.86890000
C	0.53024000	3.70727600	-1.68963500
H	1.11351800	4.53293000	-1.28240300
H	0.79631100	3.60191300	-2.74683200
N	0.98228900	2.48176800	-1.00745300
C	2.15506800	2.40120400	-0.34698200
N	2.77216400	1.20599500	-0.25330600
C	4.10441400	0.99372600	0.20548200
C	5.13685200	1.81786800	-0.25259900
C	4.39339500	-0.09566300	1.03312500
C	6.44853900	1.58080600	0.15629800
C	5.71513000	-0.33334000	1.41030500
H	3.58945800	-0.74117500	1.36645800
C	6.74803600	0.50455100	0.99005400
H	7.76998500	0.31580600	1.29721900
C	6.05109000	-1.54978200	2.23454400
C	7.54134300	2.51912300	-0.28455800
F	7.05367700	-1.29733200	3.10534600
F	6.47617400	-2.57142800	1.44507100
F	4.99776200	-2.00061200	2.93641800
F	7.29335100	3.03204700	-1.51138900
F	8.74114700	1.90171700	-0.33636200
F	7.67063000	3.56603600	0.56018100
S	2.72366200	3.78620500	0.54396000
H	4.92801900	2.62798500	-0.94043500
H	2.23016700	0.36477200	-0.46205400
H	0.52595800	1.59932700	-1.29281600
C	0.01822200	3.46462100	1.94828400
H	-0.04342700	4.48804900	2.32603100
H	1.22457500	3.66643400	1.31761100
H	0.26581700	2.68982300	2.67343900
N	-0.92894500	-0.67991800	1.50529600
S	0.54440400	-0.81484400	2.06743600
O	0.87443600	0.25460600	3.02189600
O	1.56088600	-1.13762300	1.03200800
C	0.47861800	-2.36988700	3.10011200
F	0.12508400	-3.41425400	2.34754300
F	-0.40724500	-2.24164300	4.10138100
F	1.68641000	-2.59909800	3.62759900
C	-1.82167300	3.03148400	-2.39145000
C	-2.89901700	2.30794800	-1.87210900

C	-1.53701500	2.87760600	-3.76205600
C	-3.66040200	1.46347500	-2.68465400
H	-3.16018400	2.36812200	-0.82234600
C	-2.29323000	2.03774400	-4.57549300
H	-0.71920600	3.42980600	-4.21752100
C	-3.36485700	1.32340400	-4.03686400
H	-4.48231500	0.91378000	-2.23965700
H	-2.04797900	1.94807900	-5.63070000
H	-3.95776100	0.66503900	-4.66585700
C	-1.16670800	5.46028500	-2.18357100
H	-0.49229500	6.15888200	-1.67144400
H	-0.84601800	5.42542400	-3.23329900
C	-2.57509600	5.98429500	-2.11782300
C	-2.93053100	7.12329200	-1.52108500
H	-2.20368000	7.76461200	-1.02571500
H	-3.96163100	7.46626500	-1.51476200
H	-3.33534900	5.37513200	-2.60496400
H	-0.97305800	2.07274100	0.67219100

TS-EF-3SR-1

l imaginary frequency

H = -5236.775828

G = -5236.972578

E(M06-2X-DCM) = -5237.619438

E(M06-2X-cyclohexane) = -5237.592631

O	-1.55187500	-2.45063300	-0.25240900
O	-3.04111400	-0.36222300	0.11145700
P	-1.48131000	-0.83178600	-0.01467600
O	-0.91083800	-0.08830700	-1.18478300
C	-3.28428800	-3.62858100	-3.87524500
C	-4.07578900	-3.36714800	-2.76124900
C	-3.48740400	-3.05489100	-1.52664500
C	-1.27357900	-3.18446900	-2.55100300
C	-1.89532500	-3.56702400	-3.75168000
C	-3.88122600	-0.92498400	1.07456900
C	-4.46411800	-2.16989800	0.83390600
C	-5.18883000	-2.79146400	1.86380600
C	-5.42221400	-2.13536800	3.06734200
C	-4.92850100	-0.84309800	3.24079400
C	-4.14090100	-0.21344400	2.26275800
H	-1.26665100	-3.79435500	-4.60772900
H	-5.13318600	-0.30453700	4.16134200
C	-4.55076600	-3.01831500	-0.43494600
C	-5.80698400	-2.63875200	-1.29082500

H	-5.81780300	-1.55222300	-1.43661600
H	-6.74579900	-2.91875800	-0.80302400
H	-6.68745400	-4.22232100	1.22227900
H	-5.43612800	-4.92534200	2.24160000
C	-2.10585400	-2.90277300	-1.45080000
H	-3.73535600	-3.88202400	-4.83142400
H	-5.98875800	-2.61505600	3.86150200
C	-5.58503900	-3.34456200	-2.64744300
H	-6.06200300	-2.81718000	-3.48158600
H	-6.00002700	-4.36222200	-2.64133200
C	-5.61358200	-4.18453700	1.45367000
C	-4.75700200	-4.43698200	0.19519400
H	-3.77907700	-4.83634000	0.48733500
H	-5.21046900	-5.14369700	-0.50680600
C	-3.66456600	1.18479500	2.50933900
C	-2.75350400	1.44871100	3.56153400
C	-4.20871700	2.25504900	1.75479900
C	-2.13944200	0.41092800	4.33370100
C	-2.39644900	2.81481100	3.87360000
C	-3.82662400	3.61488600	2.06529600
C	-1.26578200	0.69930400	5.34838100
H	-2.34549500	-0.62061500	4.07925800
C	-1.49057800	3.07287600	4.95015900
C	-2.93903200	3.85718800	3.11756500
C	-0.94370500	2.04771500	5.67236500
H	-0.79488400	-0.11045900	5.89780800
H	-1.24354900	4.10751400	5.17733700
H	-2.66823600	4.88382000	3.35765300
H	-0.25150800	2.25538100	6.48387400
C	0.21856800	-3.10901100	-2.47201900
C	0.92273400	-2.15795000	-3.25104200
C	0.92859400	-4.02945200	-1.66172700
C	0.26682300	-1.18639400	-4.07600900
C	2.36844900	-2.13840600	-3.22016600
C	2.37212200	-3.98138000	-1.62222500
C	0.97937400	-0.29800600	-4.84022500
H	-0.81580000	-1.15263400	-4.08071600
C	3.07389300	-1.19171800	-4.02940700
C	3.05132200	-3.04305900	-2.40328000
C	2.40440700	-0.30094600	-4.82457000
H	0.45248900	0.41877200	-5.46510000
H	4.16145400	-1.20481900	-4.00383500
H	4.13913200	-3.02090700	-2.37939400
H	2.95258900	0.40505000	-5.44293300

C	-5.65493300	3.11778700	-0.02009300
H	-6.36424000	2.93786300	-0.82314000
C	-5.15378600	2.06203700	0.69583600
H	-5.47851600	1.05472600	0.46200400
C	-5.25858900	4.45241800	0.27705300
H	-5.66760300	5.27704300	-0.30038700
C	-4.37548900	4.68939500	1.29595600
H	-4.07762700	5.70500800	1.54779100
C	0.99659800	-5.91135600	-0.10385100
H	0.47618200	-6.66572900	0.48014900
C	2.41761000	-5.84429300	-0.05281600
H	2.96806400	-6.54133700	0.57308300
C	3.08199300	-4.90752400	-0.79627800
H	4.16760000	-4.84882200	-0.77414800
C	0.28059900	-5.03973000	-0.88156400
H	-0.80017100	-5.11470800	-0.91381000
C	-0.59690100	3.67926700	-1.90199500
C	-0.99941800	3.37120400	-0.41367800
H	-1.63140100	4.20112500	-0.07116100
H	-1.62177200	2.47732300	-0.39323800
C	0.10858000	3.18777800	0.58028200
C	0.45679100	2.62028100	-2.42009700
H	1.23818400	3.13404300	-2.98251300
H	-0.03723300	1.91798700	-3.09190000
N	1.10765800	1.76804500	-1.41108600
C	2.40205600	1.80175400	-1.05560600
N	2.94072000	0.69466200	-0.51803600
C	4.26167100	0.58580200	0.01212500
C	5.36567200	0.71660600	-0.83219300
C	4.43244400	0.27806000	1.36344400
C	6.65053100	0.56183200	-0.31433200
C	5.72604400	0.11182000	1.86361400
H	3.56620100	0.18464600	2.01147700
C	6.83747100	0.25640300	1.03430000
H	7.83701800	0.12923500	1.43247700
C	5.91694200	-0.27757200	3.30835900
C	7.84380100	0.76829700	-1.21035200
F	5.83960800	-1.61667600	3.47234400
F	4.97970500	0.27648200	4.10235100
F	7.12742800	0.10826300	3.77169200
F	7.57112200	0.42713800	-2.48986800
F	8.90386400	0.03465600	-0.80909200
F	8.23887300	2.06092500	-1.22285600
S	3.26768200	3.31232500	-1.09847400

H	5.21875200	0.92240700	-1.88604300
H	2.32662300	-0.11095400	-0.31126500
H	0.56429400	0.90158400	-1.23789400
C	1.09250800	4.10558600	0.90151300
H	0.94594600	5.15154300	0.63513400
H	2.08299700	3.81955500	-0.03982000
H	1.66879800	3.92369000	1.80815500
N	-0.84341500	-0.63646100	1.45845100
S	0.66708700	-0.94511300	1.80129600
O	1.26434900	0.11032100	2.63729900
O	1.48931800	-1.40330300	0.64430900
C	0.58215900	-2.45370100	2.90172100
F	0.02581000	-3.47323500	2.24569800
F	-0.14544700	-2.19203500	3.99629800
F	1.81861600	-2.79331100	3.27886100
C	-1.86858000	3.55049300	-2.78195300
C	-2.58603400	2.33936200	-2.78334900
C	-2.33089000	4.57568900	-3.62057100
C	-3.72039700	2.17182200	-3.57502800
H	-2.25072300	1.50279400	-2.17718500
C	-3.46912200	4.40831400	-4.41515100
H	-1.81434700	5.52653400	-3.67608600
C	-4.17283600	3.20726800	-4.39480800
H	-4.24737000	1.22163100	-3.55054800
H	-3.79758800	5.22545900	-5.05230000
H	-5.05693600	3.07624100	-5.01317800
C	0.04478100	5.09282900	-2.03403700
H	1.06368100	5.06755700	-1.64145600
H	0.16762900	5.29343200	-3.10775300
C	-0.70678500	6.23452900	-1.39284500
C	-0.12606400	7.26467400	-0.77268700
H	0.95579600	7.34504700	-0.67824700
H	-0.70860800	8.07934200	-0.35113800
H	-1.79335800	6.21471800	-1.46609700
H	0.12046400	2.24025400	1.11824800

TS-EF-3SR-2

l imaginary frequency

H = -5236.771437

G = -5236.966845

E(M06-2X-DCM) = -5237.613732

E(M06-2X-cyclohexane) = -5237.586387

O	1.27929600	-2.48180500	-0.06248900
O	2.97997400	-0.54438100	-0.35869200

P	1. 38569200	-0. 84845500	-0. 14856100
O	0. 97048700	-0. 15718200	1. 11352300
C	3. 17728700	-4. 26292300	3. 21389800
C	3. 88610300	-3. 97182600	2. 05258900
C	3. 22860900	-3. 44902100	0. 92980600
C	1. 12470900	-3. 43298900	2. 16787500
C	1. 80338300	-4. 02119500	3. 24904400
C	3. 66193200	-1. 08287300	-1. 45078100
C	4. 08457900	-2. 41258700	-1. 41495200
C	4. 61946700	-2. 98799900	-2. 57927400
C	4. 83414500	-2. 22250300	-3. 71997100
C	4. 52515900	-0. 86298200	-3. 68972500
C	3. 93001500	-0. 26546900	-2. 56717700
H	1. 23448700	-4. 26887500	4. 14053700
H	4. 72948700	-0. 24124900	-4. 55657100
C	4. 17540600	-3. 41375500	-0. 26346000
C	5. 54896600	-3. 29630600	0. 48189800
H	5. 72085300	-2. 24425500	0. 73723600
H	6. 38908700	-3. 63237800	-0. 13387500
H	5. 95782200	-4. 66640900	-2. 27093200
H	4. 52760200	-5. 07292900	-3. 21328800
C	1. 87806000	-3. 12432500	1. 01956900
H	3. 68010700	-4. 67734900	4. 08414800
H	5. 25015800	-2. 66892700	-4. 61962000
C	5. 36640500	-4. 12169400	1. 77531400
H	5. 98794000	-3. 75605700	2. 60073100
H	5. 63824500	-5. 17524200	1. 61961000
C	4. 88238200	-4. 46400300	-2. 37392000
C	4. 12513700	-4. 75945300	-1. 06207600
H	3. 07835900	-4. 99616900	-1. 28435900
H	4. 54440700	-5. 59677400	-0. 49546000
C	3. 68251500	1. 21237300	-2. 58316600
C	2. 69888500	1. 76732300	-3. 43629900
C	4. 52664100	2. 06240000	-1. 82404000
C	1. 81653500	0. 96074800	-4. 22398200
C	2. 55325300	3. 20408800	-3. 52302700
C	4. 36695000	3. 49694700	-1. 91639200
C	0. 87400500	1. 52611100	-5. 04082700
H	1. 87776300	-0. 11586500	-4. 13703000
C	1. 56159200	3. 75376300	-4. 39572200
C	3. 38547200	4. 02716900	-2. 75962800
C	0. 74728700	2. 94122800	-5. 13682300
H	0. 19898700	0. 88753100	-5. 60234600
H	1. 47227300	4. 83617900	-4. 45605900

H	3.27926600	5.10788200	-2.83678400
H	-0.00502700	3.36992900	-5.79351100
C	-0.34785200	-3.18566200	2.26600000
C	-0.84550100	-2.25964100	3.21581900
C	-1.24527300	-3.93087100	1.46165100
C	0.00938800	-1.44625100	4.02916300
C	-2.27321900	-2.10227500	3.38153100
C	-2.66975000	-3.73839200	1.61316100
C	-0.50351500	-0.58183800	4.96225100
H	1.08098400	-1.51008900	3.88510500
C	-2.76661900	-1.18939900	4.36697200
C	-3.14477600	-2.84302000	2.57688700
C	-1.91120400	-0.45451300	5.14286000
H	0.17149000	0.01614100	5.56942100
H	-3.84365000	-1.09552200	4.48668700
H	-4.21923000	-2.72551100	2.70583100
H	-2.29990100	0.23012400	5.89219800
C	6.39478800	2.41547600	-0.28389500
H	7.18787800	2.00856600	0.33777500
C	5.57587300	1.56767700	-0.98387200
H	5.72749500	0.49675500	-0.91352800
C	6.22408200	3.82688400	-0.36869800
H	6.88630400	4.48563000	0.18704100
C	5.23597500	4.34731800	-1.16195800
H	5.10383000	5.42370300	-1.24814000
C	-1.70266600	-5.59431200	-0.26846900
H	-1.34120200	-6.31971500	-0.99240100
C	-3.10319700	-5.37742600	-0.13467800
H	-3.79636000	-5.92992000	-0.76306300
C	-3.57082300	-4.47849900	0.78470700
H	-4.63704800	-4.29943200	0.89394400
C	-0.80842200	-4.89922900	0.50233900
H	0.25361500	-5.08298900	0.38896300
C	1.00688200	3.46633600	2.14617300
C	1.34154200	3.26384900	0.62858100
H	2.03377300	4.05823500	0.32308100
H	1.87033700	2.31409200	0.52343400
C	0.20021000	3.27767400	-0.34702000
C	-0.14752900	2.48480900	2.56671000
H	-0.86314700	3.00219600	3.20693600
H	0.27721100	1.64937600	3.12357900
N	-0.88796800	1.83012800	1.47273200
C	-2.18744400	2.00898300	1.17456700
N	-2.83463700	0.98131700	0.60482900

C	-4.14764800	0.89753700	0.06496200
C	-4.74939700	1.89478600	-0.70680000
C	-4.81310900	-0.31266000	0.27994900
C	-6.03141500	1.68569900	-1.21473000
C	-6.08874600	-0.51165500	-0.24446800
H	-4.32504500	-1.09310000	0.85323200
C	-6.71221700	0.48891900	-0.98764500
H	-7.70584600	0.33694500	-1.39134100
C	-6.76500700	-1.84146300	-0.03300100
C	-6.71048200	2.78993900	-1.98396500
F	-6.31071500	-2.77818800	-0.89295800
F	-8.10129200	-1.76062500	-0.19600500
F	-6.53754300	-2.32131100	1.21656900
F	-7.44327200	3.58157400	-1.16728900
F	-7.55358900	2.30170900	-2.91869200
F	-5.81980600	3.58747000	-2.61136600
S	-2.88774000	3.58802900	1.38551400
H	-4.22812300	2.81580100	-0.92207500
H	-2.29838200	0.11269000	0.44907500
H	-0.42662400	0.93762300	1.20799800
C	-0.66908000	4.32385600	-0.59477500
H	-0.42001100	5.32787100	-0.25495600
H	-1.69630800	4.07212000	0.35743200
H	-1.26849100	4.27274400	-1.50294100
N	0.68052100	-0.45150600	-1.55072500
S	-0.87064400	-0.60673600	-1.81386600
O	-1.43869900	0.58557200	-2.46080600
O	-1.63627700	-1.16693000	-0.66168800
C	-0.97131300	-1.95808000	-3.09981700
F	-0.30461200	-1.59684300	-4.20726800
F	-2.25065900	-2.17064600	-3.42239500
F	-0.44292000	-3.08880600	-2.62846900
C	2.26579300	3.18064100	2.99460200
C	2.14444800	2.82076500	4.34934400
C	3.56252500	3.32640300	2.48118100
C	3.26583300	2.60422100	5.14960200
H	1.16224500	2.72057900	4.80049300
C	4.68722500	3.10749300	3.27952500
H	3.72519000	3.60014500	1.44509700
C	4.54744000	2.74386600	4.61699000
H	3.13321800	2.32562100	6.19186400
H	5.67466700	3.21680700	2.83992200
H	5.42320000	2.57084700	5.23657400
C	0.57419500	4.95829600	2.40237600

H	1.35326700	5.59878200	1.96543000
H	-0.35390400	5.15775900	1.86303800
C	0.37233800	5.35903800	3.84061700
C	-0.80902900	5.67198300	4.37858500
H	-1.73017300	5.64167300	3.80039200
H	-0.89809000	5.97582500	5.41846200
H	1.26549300	5.40708000	4.46037300
H	0.07517000	2.38181100	-0.95346700

TS-EF-3SR-3

l imaginary frequency

H = -5236.771977

G = -5236.964820

E(M06-2X-DCM) = -5237.611789

E(M06-2X-cyclohexane) = -5237.580897

O	-0.05880300	2.97516300	0.07844100
O	1.99893500	1.44805000	0.42700300
P	0.36177500	1.43620700	0.44677800
O	-0.10754800	0.44870200	-0.58205900
C	1.56267800	4.94984800	-3.23737800
C	2.22741400	4.94249000	-2.01568700
C	1.66657100	4.30927400	-0.89657700
C	-0.24385200	3.62519500	-2.25347100
C	0.32977800	4.30742600	-3.33987600
C	2.67904100	2.12087200	1.44560500
C	2.72370900	3.51290600	1.45366400
C	3.14532100	4.17165600	2.61889500
C	3.66450100	3.45066200	3.68978700
C	3.79934000	2.06490400	3.57210700
C	3.31005400	1.36885100	2.45552000
H	-0.20742800	4.31545100	-4.28393600
H	4.27987100	1.49780600	4.36425300
C	2.53471500	4.53618600	0.33614400
C	3.91974100	4.80800800	-0.35491900
H	4.39145000	3.84500400	-0.58239000
H	4.60358300	5.36962000	0.28850500
H	3.90348000	6.19613200	2.39426400
H	2.42534000	6.09807600	3.34334900
C	0.46017700	3.62480300	-1.03406200
H	1.99550700	5.44388800	-4.10357400
H	3.99465800	3.95580700	4.59407500
C	3.57559700	5.53264900	-1.67118100
H	4.32356100	5.36809100	-2.45509300
H	3.50569900	6.61986000	-1.52321300

C	2.94377500	5.66763000	2.47879100
C	2.11584800	5.78538800	1.17524500
H	1.04654800	5.71531500	1.40404000
H	2.28500400	6.72539000	0.63976800
C	3.57718800	-0.09702200	2.29761500
C	2.96407300	-1.05443200	3.13924300
C	4.53502200	-0.50852800	1.33379400
C	1.98959800	-0.70232400	4.12629100
C	3.31115600	-2.45249500	3.00575500
C	4.85769800	-1.91102200	1.19986300
C	1.42402800	-1.65169500	4.93706600
H	1.68212600	0.33223500	4.20743500
C	2.69737400	-3.41022800	3.87257800
C	4.23741500	-2.84347800	2.03618800
C	1.78602700	-3.02347900	4.81726900
H	0.67722500	-1.35798300	5.66804000
H	2.97672300	-4.45569900	3.76273500
H	4.47778100	-3.89824200	1.92565200
H	1.32774600	-3.75999500	5.47222200
C	-1.57580300	2.96829700	-2.43932500
C	-1.69309800	1.84607200	-3.29409000
C	-2.73050600	3.53543400	-1.84760200
C	-0.56093600	1.21180600	-3.90266200
C	-3.00007600	1.29644100	-3.57642200
C	-4.02885200	2.96550200	-2.12511000
C	-0.70604600	0.14659300	-4.75415000
H	0.43214700	1.57961600	-3.67259400
C	-3.11059200	0.18901300	-4.47708100
C	-4.12939500	1.86617100	-2.98213800
C	-2.00064200	-0.36632700	-5.05818000
H	0.17294000	-0.31563300	-5.19352300
H	-4.10538300	-0.18872100	-4.70602600
H	-5.11259000	1.45356300	-3.20103100
H	-2.10126100	-1.19065500	-5.76051200
C	6.15380700	-0.02102500	-0.43614500
H	6.66819500	0.70226200	-1.06342200
C	5.23515500	0.40965600	0.48545400
H	5.03754200	1.47040900	0.58561500
C	6.44649700	-1.40631200	-0.57965700
H	7.17446500	-1.73045100	-1.31861600
C	5.81745300	-2.32076500	0.22139500
H	6.03032600	-3.38176000	0.12369300
C	-3.81626300	5.22560600	-0.45754500
H	-3.74686200	6.09792100	0.18653200

C	-5.09211200	4.65441600	-0.72751400
H	-5.98298200	5.09741200	-0.29006700
C	-5.19126800	3.55720800	-1.53933300
H	-6.15879700	3.11246800	-1.75855000
C	-2.67922600	4.68739000	-0.99935300
H	-1.71712700	5.13841300	-0.78678500
C	-4.93665200	-3.04041500	0.41992800
C	-4.90570100	-3.55756900	-1.05083600
H	-4.62466400	-4.61783900	-1.08248600
H	-5.92643400	-3.49638900	-1.45725600
C	-4.02850600	-2.79027800	-1.96453900
C	-3.49358800	-3.12556200	0.99645100
H	-3.22531900	-4.18028100	1.07250000
H	-3.46446400	-2.69798000	2.00134200
N	-2.43282100	-2.45463700	0.21995800
C	-1.31742700	-3.06581800	-0.26866400
N	-0.24424400	-2.28673900	-0.47302100
C	0.96200400	-2.64982500	-1.13921800
C	1.69777800	-3.78415100	-0.78860900
C	1.43737000	-1.78116200	-2.12496400
C	2.88284000	-4.06866700	-1.46691100
C	2.63173500	-2.07292400	-2.78312600
H	0.88144600	-0.87940100	-2.35266400
C	3.35651100	-3.22118800	-2.46885000
H	4.28915600	-3.43760500	-2.97476800
C	3.10189500	-1.15789800	-3.88267200
C	3.63622700	-5.32887700	-1.13348100
F	2.48833500	-1.44837200	-5.06218800
F	4.42861800	-1.26315700	-4.09949500
F	2.82856300	0.13642300	-3.61672100
F	3.51838100	-5.65729700	0.17431100
F	4.95756400	-5.21573100	-1.40301100
F	3.18173600	-6.38588800	-1.84337800
S	-1.38224400	-4.72060000	-0.78246200
H	1.36431700	-4.42716200	0.01465500
H	-0.31603700	-1.25865000	-0.31153300
H	-2.26381000	-1.50133200	0.56489200
C	-3.22075500	-3.44320600	-2.90073600
H	-3.59852100	-4.39380700	-3.29026700
H	-2.39111100	-3.98105600	-2.11570100
H	-2.67624500	-2.83296600	-3.61944000
N	-0.09952300	1.26052200	1.98598100
S	-1.59985900	0.90191800	2.33177600
O	-1.88927100	-0.56159600	2.26739200

O	-2.63296100	1.77007300	1.74044600
C	-1.63834400	1.30835000	4.15056100
F	-0.74395000	0.59802000	4.84830700
F	-2.86202200	1.02097600	4.61428500
F	-1.39888300	2.60704100	4.33787400
C	-5.59632600	-1.64941900	0.45610700
C	-6.89372700	-1.49259400	-0.07107700
C	-4.98089800	-0.52036100	1.00829000
C	-7.54353400	-0.26119800	-0.04689800
H	-7.42158700	-2.34283100	-0.49741300
C	-5.62308100	0.72235700	1.02076000
H	-3.99553200	-0.57601000	1.45308100
C	-6.90624500	0.85632600	0.49775700
H	-8.54781000	-0.17678900	-0.45443900
H	-5.09069800	1.57287100	1.43262100
H	-7.40660300	1.82063500	0.51215500
C	-5.79681000	-4.05394600	1.24908400
H	-5.37578000	-5.06093800	1.12853700
H	-6.80346200	-4.07928500	0.81049300
C	-5.90633400	-3.72724300	2.71486300
C	-5.54128700	-4.54731200	3.70139700
H	-5.11886700	-5.53116700	3.50533400
H	-5.65519900	-4.26864900	4.74530900
H	-3.98794400	-1.70761400	-1.86346200
H	-6.32446700	-2.75073100	2.95636700

TS-EF-3SR-4

l imaginary frequency

H = -5236.774000

G = -5236.965323

E(M06-2X-DCM) = -5237.617008

E(M06-2X-cyclohexane) = -5237.585961

O	0.12868900	2.92877400	-0.11971500
O	-1.99871200	1.49173000	-0.45063200
P	-0.36331300	1.41712000	-0.52740700
O	0.09505200	0.39052800	0.46624400
C	-1.30847600	4.78929100	3.34965200
C	-2.02535600	4.84838300	2.15956400
C	-1.52592300	4.25872200	0.98812700
C	0.42776900	3.48287000	2.22694600
C	-0.08334400	4.12504800	3.36730700
C	-2.67669300	2.22882300	-1.42752300
C	-2.68831400	3.61993600	-1.35917700
C	-3.11971500	4.35430400	-2.47418900

C	-3.66899100	3.70769100	-3.57659800
C	-3.81957500	2.31975600	-3.54101400
C	-3.32677800	1.54990100	-2.47551100
H	0.49665200	4.08338000	4.28480700
H	-4.31251700	1.80688400	-4.36186800
C	-2.43813700	4.57134800	-0.19286900
C	-3.78779300	4.83270600	0.56671200
H	-4.27152300	3.86841800	0.76081100
H	-4.48345800	5.44219000	-0.01778500
H	-3.83462100	6.37267400	-2.10349500
H	-2.38923400	6.30978100	-3.10505100
C	-0.32898400	3.54565300	1.04039900
H	-1.69421900	5.25013700	4.25547000
H	-4.00417900	4.27093700	-4.44391100
C	-3.37540200	5.47849600	1.90406100
H	-4.09251100	5.28372500	2.70959700
H	-3.29104900	6.57082800	1.81260400
C	-2.88753700	5.83530600	-2.25182700
C	-2.01786300	5.85929500	-0.97158300
H	-0.95820300	5.77994200	-1.23931200
H	-2.14782400	6.76961600	-0.37704500
C	-3.60542600	0.07833000	-2.42833100
C	-2.98057200	-0.81608400	-3.32889300
C	-4.59284500	-0.39454500	-1.52570200
C	-1.96933500	-0.39985900	-4.25229900
C	-3.35232500	-2.21459000	-3.32170400
C	-4.94435400	-1.79670900	-1.52134300
C	-1.38564200	-1.28977900	-5.11603900
H	-1.63588400	0.63001500	-4.23784500
C	-2.72552800	-3.10725300	-4.24666600
C	-4.31426800	-2.66724300	-2.41538500
C	-1.77464100	-2.65940500	-5.12370700
H	-0.59793100	-0.94681600	-5.77889300
H	-3.02487200	-4.15305500	-4.23475500
H	-4.58169000	-3.72141600	-2.40521300
H	-1.30438000	-3.34814400	-5.82105600
C	1.75633300	2.80151200	2.32243500
C	1.89697900	1.63554500	3.11259400
C	2.89055800	3.38386200	1.70710200
C	0.78815700	0.99864500	3.75982900
C	3.20466900	1.04484400	3.28816500
C	4.18884200	2.77310000	1.87686100
C	0.95780700	-0.10979800	4.54949700
H	-0.20658400	1.40373600	3.61496000

C	3.34061900	-0.11227300	4.12033700
C	4.31156600	1.62235700	2.66034100
C	2.25415600	-0.66970800	4.74269600
H	0.09577600	-0.56692800	5.02666800
H	4.33753500	-0.52330500	4.26801400
H	5.29355000	1.17187200	2.79008200
H	2.37682800	-1.52916000	5.39792700
C	-6.25200800	-0.02497700	0.23506600
H	-6.76974200	0.65263200	0.90901600
C	-5.29748700	0.46276900	-0.61931300
H	-5.07288200	1.52309800	-0.62042800
C	-6.57828800	-1.41036100	0.24700000
H	-7.33647600	-1.78102500	0.93180200
C	-5.94200800	-2.26693100	-0.61049100
H	-6.18322800	-3.32619300	-0.61451000
C	3.93458700	5.13112300	0.35503000
H	3.84978300	6.04295500	-0.22984800
C	5.20973000	4.51764000	0.51470500
H	6.08432500	4.96626500	0.05114000
C	5.32919800	3.37426100	1.25738800
H	6.29759100	2.90040600	1.39752500
C	2.81829600	4.58584400	0.93220600
H	1.85660300	5.06949400	0.80609700
C	4.61591600	-3.41062600	-0.55996900
C	4.51645400	-4.08272100	0.84217700
H	4.11477800	-5.09984700	0.75101100
H	5.53102900	-4.19275800	1.25181700
C	3.72103600	-3.33272700	1.84266600
C	3.17202100	-3.28774800	-1.12557800
H	2.80068800	-4.29580800	-1.31836900
H	3.17065500	-2.73672000	-2.06884100
N	2.18836300	-2.61852600	-0.25206300
C	1.00208800	-3.16790400	0.14261000
N	-0.00299600	-2.31632700	0.38178700
C	-1.21767100	-2.59251800	1.07542600
C	-2.06889000	-3.64277900	0.72538300
C	-1.56978500	-1.71628600	2.10494300
C	-3.24535700	-3.83926200	1.44959000
C	-2.75453200	-1.92013900	2.81085600
H	-0.92188100	-0.87867000	2.33414900
C	-3.59502600	-2.98675800	2.49683000
H	-4.51904400	-3.13729200	3.04086700
C	-3.07865200	-1.00389700	3.96060800
C	-4.12098200	-5.01829900	1.11639100

F	-2.37971200	-1.34860700	5.07635700
F	-4.38460600	-1.04197100	4.29193400
F	-2.75855100	0.27933100	3.69005700
F	-4.13566900	-5.27611100	-0.21251700
F	-5.40097300	-4.82653000	1.50487000
F	-3.68923200	-6.14609100	1.72591900
S	0.90733300	-4.86091200	0.49976500
H	-1.83031300	-4.28807000	-0.10902600
H	0.14904200	-1.29123200	0.23800600
H	2.12682100	-1.61339800	-0.45103800
C	2.85633300	-4.00037900	2.71393000
H	3.13656800	-5.02001600	2.99567000
H	1.97529100	-4.37187500	1.88053900
H	2.37251300	-3.42200800	3.49894200
N	0.01941800	1.31742900	-2.08888700
S	1.30788900	0.70571300	-2.75059300
O	1.16177800	0.59221500	-4.20170500
O	1.87881000	-0.47033900	-2.03410200
C	2.63074200	2.00707700	-2.52606300
F	2.23780900	3.18224800	-3.01743800
F	3.75222300	1.62583600	-3.16388800
F	2.92058700	2.15212300	-1.22326700
C	5.41514000	-2.09901000	-0.45528700
C	6.68131100	-2.12011400	0.16139500
C	4.97717300	-0.88297100	-0.99361500
C	7.47365300	-0.97797800	0.24168100
H	7.07808100	-3.04497600	0.57315200
C	5.76811500	0.26802300	-0.90910300
H	4.02299200	-0.80348600	-1.50165900
C	7.01630300	0.22712200	-0.29413300
H	8.44902700	-1.03327700	0.71828800
H	5.39540000	1.19461600	-1.32928900
H	7.63067900	1.12162400	-0.23841300
C	5.38575200	-4.41131300	-1.49435500
H	4.85831500	-5.37656500	-1.45672900
H	6.38273700	-4.57973700	-1.07261500
C	5.52488900	-3.97655400	-2.92994800
C	6.68113000	-3.65900900	-3.51231400
H	7.62268200	-3.68276300	-2.96769700
H	6.73028400	-3.35866000	-4.55515700
H	3.79148200	-2.24742600	1.86402400
H	4.61045800	-3.93803500	-3.52148000

TS-EF-3RS

l imaginary frequency

H = -5236.777802

G = -5236.971142

E(M06-2X-DCM) = -5237.617108

E(M06-2X-cyclohexane) = -5237.588825

O	0.22136400	-2.91452500	0.04511400
O	2.38653600	-1.52382600	-0.17619900
P	0.76350500	-1.37854000	-0.14337700
O	0.41812300	-0.50201400	1.02151100
C	1.44383000	-4.96263800	3.48723200
C	2.23358800	-4.96160700	2.34222300
C	1.79522600	-4.32773400	1.16955400
C	-0.23112800	-3.60865600	2.32739100
C	0.21239600	-4.30806400	3.46212700
C	2.99902100	-2.25036600	-1.19925400
C	3.03840600	-3.64166700	-1.12816400
C	3.48443700	-4.36664800	-2.24473500
C	4.00509300	-3.71051400	-3.35509900
C	4.08435200	-2.31720700	-3.34493600
C	3.57287500	-1.55535100	-2.28190300
H	-0.41943800	-4.31005900	4.34567500
H	4.52899200	-1.79436500	-4.18659900
C	2.76852700	-4.60305800	0.02792900
C	4.08166000	-4.86014800	0.84621600
H	4.53628000	-3.89358500	1.09218600
H	4.81809600	-5.44088000	0.28244500
H	4.25268500	-6.35760400	-1.84274000
H	2.83716400	-6.34759100	-2.88858100
C	0.59575800	-3.61928000	1.18786400
H	1.77931100	-5.45987200	4.39390200
H	4.35906100	-4.27080300	-4.21694600
C	3.61046800	-5.55472800	2.14124600
H	4.27792200	-5.36702900	2.98998400
H	3.55959100	-6.64552500	2.01495800
C	3.29347600	-5.85248500	-2.02368300
C	2.38970700	-5.89370800	-0.77069300
H	1.33736200	-5.82618700	-1.06947600
H	2.51194400	-6.80475300	-0.17614300
C	3.69187100	-0.06395500	-2.30414200
C	3.02308300	0.69305700	-3.29739600
C	4.53712200	0.58203000	-1.36596400
C	2.13979800	0.10606500	-4.25997700
C	3.20855000	2.12649900	-3.34707200
C	4.68895500	2.01863000	-1.41135700

C	1. 52360900	0. 86606500	-5. 21857900
H	1. 93120600	-0. 95489900	-4. 20036400
C	2. 54915100	2. 88221800	-4. 36688900
C	4. 02262300	2. 75033300	-2. 39817000
C	1. 73761200	2. 27190600	-5. 28414900
H	0. 84389700	0. 39482800	-5. 92260300
H	2. 71169400	3. 95747300	-4. 39463400
H	4. 13468900	3. 83217700	-2. 42369600
H	1. 24300000	2. 85649000	-6. 05563800
C	-1. 54618800	-2. 89635300	2. 37287500
C	-1. 70755800	-1. 77414800	3. 22156200
C	-2. 64219700	-3. 38384200	1. 62054300
C	-0. 62557900	-1. 20506500	3. 96955900
C	-3. 00403800	-1. 14591900	3. 33694500
C	-3. 92712600	-2. 73121700	1. 72529700
C	-0. 81247100	-0. 12141600	4. 78836800
H	0. 36261900	-1. 63546800	3. 86311200
C	-3. 15968400	-0. 02408000	4. 21253500
C	-4. 07630400	-1. 64084500	2. 58798200
C	-2. 09990100	0. 47516500	4. 92088100
H	0. 03079800	0. 29286200	5. 33528600
H	-4. 14731700	0. 42338600	4. 30407000
H	-5. 05346800	-1. 16996400	2. 67955700
H	-2. 23320200	1. 32743700	5. 58200900
C	6. 07881200	0. 52916100	0. 53299100
H	6. 62566500	-0. 03690500	1. 28218000
C	5. 28040700	-0. 12633300	-0. 36714500
H	5. 21004400	-1. 20722800	-0. 33000300
C	6. 20234000	1. 94678100	0. 49885900
H	6. 83656100	2. 44927400	1. 22429800
C	5. 53044100	2. 66592900	-0. 45218900
H	5. 61463500	3. 74891600	-0. 49194500
C	-3. 62503500	-4. 97044400	0. 04409800
H	-3. 52205300	-5. 83683600	-0. 60371000
C	-4. 88300400	-4. 31016000	0. 13605300
H	-5. 72544700	-4. 67418700	-0. 44599600
C	-5. 02731100	-3. 22462700	0. 95654400
H	-5. 98202100	-2. 71009400	1. 03476900
C	-2. 54635700	-4. 52505800	0. 76165600
H	-1. 59735900	-5. 04278900	0. 68322100
N	0. 32497500	-0. 96299700	-1. 64429100
S	-1. 14694600	-0. 71830900	-2. 13980900
O	-1. 22285600	0. 35270500	-3. 14774200
O	-2. 17517200	-0. 65760700	-1. 05810100

C	-1.58803300	-2.26459800	-3.09206300
F	-0.72154200	-2.43950300	-4.09750600
F	-2.81965000	-2.13532900	-3.60277800
F	-1.55684200	-3.33707000	-2.29935900
C	-4.93464800	2.17221700	-0.47240700
C	-4.21849200	2.11520600	-1.85707500
H	-4.91526800	2.51111100	-2.60947800
H	-4.01632100	1.06999300	-2.10158300
C	-2.93077800	2.86649000	-2.00134400
C	-3.91653200	1.76312000	0.66229800
H	-4.05328800	2.40583000	1.53380400
H	-4.11550300	0.73235800	0.96264400
N	-2.48885600	1.77870800	0.30662700
C	-1.55034100	2.59889200	0.83370300
N	-0.32242800	2.09316000	0.99653800
C	0.86179800	2.78616200	1.37487700
C	1.33098100	3.90405900	0.68447400
C	1.60385600	2.24641900	2.42966400
C	2.52650000	4.50308700	1.08254800
C	2.79733200	2.85378400	2.81342400
H	1.24331000	1.35762300	2.93433600
C	3.26152300	3.98976500	2.15027800
H	4.19029000	4.45852400	2.45161500
C	3.62480500	2.24926500	3.91816500
C	3.00694900	5.73487800	0.36173400
F	2.86576900	1.53894800	4.78270600
F	4.56906800	1.41260500	3.43761200
F	4.26872200	3.20157200	4.63061400
F	2.45125100	6.86010100	0.86328400
F	4.34849300	5.88331100	0.45449400
F	2.69531300	5.69771500	-0.95485000
S	-1.95263500	4.26078100	1.13344900
H	0.78298300	4.29306900	-0.16374000
H	-0.19241500	1.05384300	0.96455200
H	-2.16610500	0.86645000	-0.05541800
C	-2.74172500	4.22689800	-1.81687100
H	-3.60881600	4.88575100	-1.81389200
H	-2.44699900	4.29317000	-0.47364700
H	-1.82921400	4.66370100	-2.22272400
C	-5.50386200	3.59712500	-0.15748600
H	-4.68819500	4.29980900	0.02952100
H	-6.04502900	3.51710800	0.79553100
C	-6.11973000	1.18117800	-0.43643500
C	-6.58829300	0.48894900	-1.56099400

C	-6.78881500	0.96510800	0.78251600
C	-7.67518300	-0.38575800	-1.47240900
H	-6.10992500	0.61374500	-2.52561900
C	-7.87101300	0.09187500	0.87627500
H	-6.46388300	1.48666900	1.67943700
C	-8.32175000	-0.59048600	-0.25582500
H	-8.01057900	-0.90836600	-2.36408000
H	-8.36480900	-0.05032700	1.83397100
H	-9.16725700	-1.26937000	-0.18852000
C	-6.44415200	4.15120400	-1.19366900
C	-6.39498500	5.39138200	-1.68507600
H	-5.64280200	6.11027100	-1.36426300
H	-7.12001000	5.74677500	-2.41219700
H	-7.23285400	3.47930800	-1.53254200
H	-2.08290200	2.26773800	-2.33259300

TS-EF-3RS-1

l imaginary frequency

H = -5236.773922

G = -5236.966676

E(M06-2X-DCM) = -5237.613115

E(M06-2X-cyclohexane) = -5237.585177

O	-0.04992200	2.89440900	0.15340700
O	-2.26136300	1.60998100	-0.21032500
P	-0.64833600	1.39430400	-0.12884400
O	-0.37929800	0.44345300	0.99548600
C	-1.34707400	4.86736200	3.61260400
C	-2.07828000	4.94699400	2.43208900
C	-1.61361600	4.33559400	1.25751200
C	0.31914000	3.47966600	2.48089500
C	-0.14755200	4.15579200	3.62032700
C	-2.80559800	2.39591200	-1.22789600
C	-2.78330100	3.78415100	-1.11350500
C	-3.15095100	4.56274200	-2.22237600
C	-3.65941500	3.96527500	-3.37103700
C	-3.80730100	2.57760600	-3.40668100
C	-3.37312400	1.76119900	-2.34994900
H	0.43965000	4.09478100	4.53211600
H	-4.24631300	2.10240600	-4.27902200
C	-2.51933000	4.69519600	0.08362800
C	-3.85580000	4.98767800	0.85128200
H	-4.36579800	4.03635800	1.04187700
H	-4.53745500	5.62173200	0.27621200
H	-3.83889700	6.57667200	-1.78954700

H	-2.38187900	6.52755300	-2.77528700
C	-0.44962300	3.57094000	1.30493500
H	-1.70365900	5.34624900	4.52106300
H	-3.95297300	4.56704400	-4.22758300
C	-3.41381900	5.61430800	2.19011500
H	-4.12897700	5.43208100	3.00027500
H	-3.30411900	6.70479000	2.10497400
C	-2.89829600	6.03024600	-1.94619000
C	-2.04782100	5.99038700	-0.65580900
H	-0.98772700	5.88314200	-0.91258500
H	-2.15425000	6.88752200	-0.03752300
C	-3.56529500	0.27860800	-2.41373100
C	-2.89704400	-0.49077600	-3.39763700
C	-4.47413600	-0.34387300	-1.51982300
C	-1.95296200	0.07151600	-4.31632600
C	-3.14704900	-1.91290000	-3.48238600
C	-4.69133900	-1.77048800	-1.59956200
C	-1.33746000	-0.69900100	-5.26701700
H	-1.69975200	1.12086200	-4.22920200
C	-2.48576800	-2.68012100	-4.49246900
C	-4.02346300	-2.51487600	-2.57585400
C	-1.61333400	-2.09205300	-5.36756700
H	-0.61225700	-0.24739400	-5.93768600
H	-2.69804500	-3.74562300	-4.54847200
H	-4.18429600	-3.58971700	-2.62574300
H	-1.11909800	-2.68489600	-6.13303400
C	1.60168900	2.71206700	2.56128100
C	1.67209400	1.54027300	3.35289000
C	2.75960400	3.20211000	1.91062500
C	0.52984400	0.98106300	4.01327300
C	2.93467500	0.85261900	3.50212700
C	4.01502700	2.50345800	2.06477000
C	0.62881200	-0.15210300	4.77858000
H	-0.43238800	1.46139100	3.88416300
C	2.99635600	-0.32521400	4.31325600
C	4.06960300	1.35192900	2.85594200
C	1.88065400	-0.81458300	4.93720900
H	-0.25842200	-0.55638400	5.25909700
H	3.95723400	-0.82299900	4.42470100
H	5.02227300	0.84047500	2.98254200
H	1.94255300	-1.70905300	5.55134500
C	-6.07876500	-0.25320500	0.32488800
H	-6.62497000	0.32421600	1.06581000
C	-5.21882500	0.38022300	-0.53341900

H	-5.09944500	1.45565200	-0.47183300
C	-6.26766100	-1.66229700	0.25718700
H	-6.95135500	-2.14762500	0.94862100
C	-5.59644200	-2.39479500	-0.68414400
H	-5.73093700	-3.47140500	-0.74861400
C	3.89715200	4.85309600	0.51285900
H	3.86448900	5.75963000	-0.08538500
C	5.13075400	4.15848500	0.66556000
H	6.02773100	4.54321000	0.18714500
C	5.18412800	3.01823300	1.42154500
H	6.12031600	2.48038400	1.54981000
C	2.75625400	4.39329800	1.11611900
H	1.82781900	4.94003100	0.99779000
N	-0.17128400	1.03998500	-1.63680100
S	1.30428600	0.71814100	-2.06721100
O	1.37093700	-0.30934700	-3.12033500
O	2.26026500	0.53458600	-0.93154400
C	1.91202800	2.27245200	-2.90761100
F	1.13759700	2.54930100	-3.96272900
F	3.16886300	2.08403800	-3.33030900
F	1.88762000	3.30612600	-2.06464800
C	4.76224400	-2.58855800	-0.75739600
C	3.95144400	-2.53612400	-2.11564100
H	4.58921500	-3.00899100	-2.87562700
H	3.83431100	-1.49057200	-2.40349100
C	2.59601400	-3.16704700	-2.17004200
C	3.83220400	-2.18858100	0.45344900
H	3.93788600	-2.93006600	1.24397400
H	4.14114000	-1.22325700	0.85890300
N	2.39547000	-2.05166500	0.16143900
C	1.40845500	-2.79669500	0.71511400
N	0.22644200	-2.19449100	0.90366900
C	-1.00744100	-2.79677600	1.27865500
C	-1.55231400	-3.88109800	0.58988600
C	-1.71880200	-2.19805800	2.32272800
C	-2.79159100	-4.38956100	0.97922500
C	-2.95771800	-2.71395000	2.69678300
H	-1.30014500	-1.33395900	2.82474000
C	-3.49783000	-3.81743600	2.03630800
H	-4.46153700	-4.21471400	2.33040400
C	-3.75256200	-2.03977500	3.78484700
C	-3.35137500	-5.58709200	0.25840500
F	-2.95478600	-1.38565700	4.65992200
F	-4.61920000	-1.13385200	3.28422400

F	-4.48151300	-2.93341600	4.49115800
F	-2.86953500	-6.74656500	0.75802700
F	-4.69952800	-5.64851300	0.35010400
F	-3.03752000	-5.56936900	-1.05894200
S	1.68074300	-4.48380700	1.01354400
H	-1.02771500	-4.31489100	-0.25109700
H	0.17527800	-1.15002500	0.88566200
H	2.14362500	-1.09870000	-0.14864300
C	2.28985500	-4.50920600	-1.97596600
H	3.08623000	-5.24986100	-2.04593500
H	2.08092300	-4.56070400	-0.64691800
H	1.31789100	-4.85354700	-2.33022600
C	5.27309300	-4.03584000	-0.51637200
H	5.82561000	-4.38088400	-1.40266400
H	4.39813700	-4.69215900	-0.45667300
C	5.91156600	-1.57376900	-0.95712100
C	5.63548700	-0.19498500	-0.95683100
C	7.22280000	-1.97650400	-1.24961700
C	6.63572400	0.74095800	-1.21946000
H	4.62649100	0.16733600	-0.77985300
C	8.22549500	-1.04020500	-1.51142000
H	7.48654600	-3.02755400	-1.25865500
C	7.93842300	0.32345700	-1.49521100
H	6.38390000	1.79747100	-1.21126800
H	9.23348900	-1.38493600	-1.72700300
H	8.71844600	1.05179500	-1.70033300
C	6.10103700	-4.34551900	0.71173200
C	6.59394000	-3.51969600	1.63611200
H	6.47036800	-2.44209600	1.59382000
H	7.16182700	-3.90629400	2.47805400
H	6.28799100	-5.41384100	0.83294300
H	1.78517300	-2.48765200	-2.42976100

TS-EF-3RS-2

l imaginary frequency

H = -5236.772627

G = -5236.964743

E(M06-2X-DCM) = -5237.607262

E(M06-2X-cyclohexane) = -5237.578305

O	0.00666800	3.02177500	-0.06209400
O	2.17949500	1.62658800	0.23971400
P	0.55319300	1.50769600	0.24048300
O	0.19220000	0.55479100	-0.85958800
C	1.28442200	4.98652000	-3.53123100

C	2. 04315000	5. 03091300	-2. 36641500
C	1. 59104100	4. 41259100	-1. 19055600
C	-0. 39249200	3. 62794200	-2. 38024600
C	0. 06804200	4. 30461200	-3. 52181800
C	2. 83549800	2. 38310900	1. 21146500
C	2. 83204000	3. 77398900	1. 12858900
C	3. 29013900	4. 51892400	2. 22680300
C	3. 88668400	3. 88620700	3. 31264600
C	4. 03976700	2. 49880500	3. 28999800
C	3. 50919000	1. 71387000	2. 25292000
H	-0. 54054200	4. 27072200	-4. 42093200
H	4. 56315000	1. 99961500	4. 10014200
C	2. 53568100	4. 72228400	-0. 03313100
C	3. 85805400	5. 00377600	-0. 83205900
H	4. 34185500	4. 04604500	-1. 05662000
H	4. 56887100	5. 60957200	-0. 26218000
H	3. 96942000	6. 54351600	1. 82774300
H	2. 55892200	6. 46631200	2. 87724100
C	0. 40384600	3. 68363300	-1. 22053000
H	1. 63231100	5. 47067800	-4. 44027000
H	4. 25340500	4. 46135500	4. 15916600
C	3. 39656300	5. 66734300	-2. 14515900
H	4. 08824800	5. 49004400	-2. 97656100
H	3. 30916900	6. 75747700	-2. 03362700
C	3. 03392900	5. 99600700	2. 00862300
C	2. 12203500	6. 00461100	0. 75902500
H	1. 07336300	5. 90886100	1. 06190000
H	2. 21783600	6. 91565600	0. 15952500
C	3. 73231900	0. 23381500	2. 23428600
C	3. 22672400	-0. 58799400	3. 27239200
C	4. 52897700	-0. 33576700	1. 20614800
C	2. 42063400	-0. 08141000	4. 34189000
C	3. 51454100	-2. 00578300	3. 26868600
C	4. 77911000	-1. 75950200	1. 19906000
C	1. 98124000	-0. 89604200	5. 35285100
H	2. 13788300	0. 96389500	4. 33200800
C	3. 03051900	-2. 82169500	4. 33904000
C	4. 26240300	-2. 55538500	2. 22472400
C	2. 29704600	-2. 28394500	5. 36160700
H	1. 36506300	-0. 48193800	6. 14565900
H	3. 26908600	-3. 88284400	4. 32304000
H	4. 44806700	-3. 62730300	2. 21048900
H	1. 94359600	-2. 91245400	6. 17498400
C	-1. 70001900	2. 90154300	-2. 44368400

C	-1.81806400	1.73219000	-3.23293800
C	-2.83462700	3.43405800	-1.78522500
C	-0.70453100	1.14000400	-3.91321300
C	-3.10382200	1.08492400	-3.36441900
C	-4.11453100	2.77746300	-1.92464500
C	-0.85086000	0.01271700	-4.67989300
H	0.27303800	1.59386900	-3.80309300
C	-3.21385400	-0.09160300	-4.17243200
C	-4.21464200	1.62317100	-2.70751400
C	-2.12399100	-0.61342500	-4.81558200
H	0.01396000	-0.41413700	-5.18106800
H	-4.19110200	-0.55995900	-4.26787500
H	-5.18428300	1.14139100	-2.81992100
H	-2.22292600	-1.50482700	-5.42935600
C	5.89244200	-0.14093400	-0.81659700
H	6.33563400	0.47663900	-1.59296600
C	5.13543400	0.44063700	0.16614200
H	4.99706500	1.51527400	0.16560300
C	6.10776700	-1.54762500	-0.83374000
H	6.70541100	-1.99084700	-1.62564300
C	5.56971500	-2.32973800	0.15169300
H	5.72623300	-3.40542400	0.15517100
C	-3.90231700	5.12991000	-0.38738800
H	-3.83237900	6.03455500	0.21008400
C	-5.16031200	4.47794200	-0.52690200
H	-6.03878000	4.89524500	-0.04164500
C	-5.25986900	3.33582800	-1.27516800
H	-6.21483700	2.82942000	-1.39231500
C	-2.78283000	4.62782500	-0.99639800
H	-1.83426100	5.14000000	-0.88412000
N	0.10009000	1.21905900	1.76441200
S	-1.40353500	1.26589400	2.24538000
O	-2.32401200	0.42168000	1.41945100
O	-1.92994800	2.57032100	2.65147500
C	-1.27526700	0.28953100	3.82588800
F	-0.71295500	-0.91337300	3.61063400
F	-2.51643400	0.08418500	4.29814800
F	-0.56994800	0.94138200	4.75093600
C	-4.85944000	-2.35077000	0.71952400
C	-4.08716600	-2.46852500	2.09324900
H	-4.76436500	-2.98341500	2.78872600
H	-3.92751600	-1.46089400	2.48037300
C	-2.76990600	-3.17622000	2.09403700
C	-3.87591100	-1.89058600	-0.41977300

H	-4.02021200	-2.52741000	-1.29249600
H	-4.09599900	-0.86607400	-0.72247000
N	-2.43979300	-1.90465600	-0.08333000
C	-1.49570400	-2.64346800	-0.72060700
N	-0.28977700	-2.08300800	-0.86785400
C	0.89345900	-2.70874900	-1.35221100
C	1.45338800	-3.82282600	-0.72618500
C	1.53908700	-2.11166400	-2.43810000
C	2.64442100	-4.35849400	-1.21584600
C	2.72665800	-2.66026800	-2.91916800
H	1.10569000	-1.22860100	-2.89328400
C	3.28207600	-3.78925400	-2.31776600
H	4.20699700	-4.21004800	-2.69261400
C	3.44931400	-1.99573300	-4.06241800
C	3.23096700	-5.57737800	-0.55429400
F	2.59531400	-1.34798700	-4.88810500
F	4.34619200	-1.08446500	-3.62834600
F	4.12989100	-2.89477500	-4.80782300
F	2.70422300	-6.72104600	-1.04407300
F	4.57010600	-5.65195800	-0.73226900
F	3.00139000	-5.58008300	0.78003500
S	-1.85027600	-4.28052800	-1.16449400
H	0.97744900	-4.25597700	0.14435900
H	-0.20590700	-1.03933900	-0.78413400
H	-2.12271400	-1.01545400	0.33491800
C	-2.54296900	-4.51620000	1.79254200
H	-3.38824900	-5.20386600	1.79666900
H	-2.30593800	-4.47764000	0.47733400
H	-1.60328000	-4.95058000	2.13463000
C	-5.44764500	-3.73933000	0.30884800
H	-6.05821900	-4.12407100	1.13713800
H	-4.62315800	-4.44433900	0.18037100
C	-5.96988300	-1.30423400	0.97665700
C	-5.65004700	0.06338200	1.03949200
C	-7.29245800	-1.67477600	1.26712100
C	-6.61802100	1.01862300	1.34975900
H	-4.63026000	0.40155300	0.88320900
C	-8.26398000	-0.71938400	1.57431600
H	-7.58980600	-2.71761100	1.26100900
C	-7.93334200	0.63369900	1.61162800
H	-6.32988000	2.06495300	1.38911800
H	-9.27999800	-1.04160100	1.78712800
H	-8.68802400	1.37774000	1.85186700
C	-6.25637100	-3.74317000	-0.96559900

C	-5.97783700	-4.50050700	-2.02878200
H	-5.12027600	-5.16959000	-2.05080400
H	-6.60039500	-4.48035100	-2.91945300
H	-7.12136700	-3.08376700	-1.00141000
H	-1.91653500	-2.58332500	2.41320800

TS-EF-3RS-3

1 imaginary frequency

H = -5236.774497

G = -5236.968286

E(M06-2X-DCM) = -5237.613533

E(M06-2X-cyclohexane) = -5237.585161

O	0.19753800	-2.90572200	0.18509000
O	2.37194000	-1.53262800	-0.05156900
P	0.74877200	-1.38614600	-0.08934700
O	0.36121700	-0.43050800	0.99700500
C	1.31194900	-4.73658200	3.78326300
C	2.13340700	-4.81083700	2.66326100
C	1.73270800	-4.24896200	1.44140700
C	-0.32098100	-3.45041400	2.49384600
C	0.08616000	-4.07876500	3.68242900
C	3.01971500	-2.32000500	-1.00556200
C	3.04887100	-3.70488400	-0.85273100
C	3.52796800	-4.49509900	-1.90971500
C	4.09131300	-3.90637000	-3.03691700
C	4.18121300	-2.51514900	-3.10298200
C	3.63792600	-1.69115200	-2.10403900
H	-0.57031600	-4.02236000	4.54599500
H	4.66004400	-2.04377100	-3.95621500
C	2.73743500	-4.59634500	0.34787000
C	4.02437800	-4.81024100	1.21884600
H	4.47823100	-3.83292200	1.41961300
H	4.77298000	-5.42757200	0.71298000
H	4.26857700	-6.46414500	-1.37040900
H	2.88668300	-6.50602300	-2.45938400
C	0.53719100	-3.53613400	1.38092600
H	1.61857300	-5.17798400	4.72823400
H	4.47081000	-4.51689600	-3.85252900
C	3.51098100	-5.42285200	2.53880600
H	4.15514300	-5.18851900	3.39391200
H	3.45532400	-6.51896200	2.47641000
C	3.31929800	-5.96481000	-1.61006300
C	2.37610100	-5.92954100	-0.38603100
H	1.33408000	-5.87531800	-0.72141200

H	2. 47440900	-6. 80499600	0. 26387600
C	3. 77168600	-0. 20424000	-2. 20370200
C	3. 14811400	0. 50226600	-3. 26145800
C	4. 58754500	0. 48582800	-1. 27073700
C	2. 29473600	-0. 12972600	-4. 22252600
C	3. 35080900	1. 92909500	-3. 38332300
C	4. 75623100	1. 91631100	-1. 38963400
C	1. 72297500	0. 58099100	-5. 24442200
H	2. 07268000	-1. 18385300	-4. 11194600
C	2. 73809600	2. 63251900	-4. 46765700
C	4. 13563400	2. 59765400	-2. 44029600
C	1. 95472000	1. 97903400	-5. 37971800
H	1. 06482500	0. 07723700	-5. 94636700
H	2. 91361800	3. 70302200	-4. 54903700
H	4. 26075400	3. 67525000	-2. 52161300
H	1. 49604900	2. 52389800	-6. 20093100
C	-1. 63286900	-2. 73216500	2. 45603900
C	-1. 81167500	-1. 55550000	3. 22339100
C	-2. 70960300	-3. 26485400	1. 70669000
C	-0. 74890000	-0. 94356800	3. 96496000
C	-3. 10651300	-0. 91444800	3. 25720600
C	-3. 99306600	-2. 60159500	1. 73008200
C	-0. 95271600	0. 19320200	4. 70387300
H	0. 23886200	-1. 38559400	3. 91867700
C	-3. 28046800	0. 26475700	4. 05000000
C	-4. 15939100	-1. 45444200	2. 51217000
C	-2. 23907100	0. 80447000	4. 75583200
H	-0. 12301100	0. 63904400	5. 24661100
H	-4. 26653400	0. 72386900	4. 07973700
H	-5. 13613100	-0. 97521800	2. 54603400
H	-2. 38607000	1. 70026900	5. 35344600
C	6. 05473900	0. 52602700	0. 68676700
H	6. 56648900	-0. 00203800	1. 48677900
C	5. 28481900	-0. 17193300	-0. 20623100
H	5. 20207800	-1. 24845300	-0. 11211700
C	6. 19459900	1. 93839300	0. 57888900
H	6. 80631600	2. 47528200	1. 29904200
C	5. 56736900	2. 60897600	-0. 43604400
H	5. 66472500	3. 68722400	-0. 53256400
C	-3. 65606800	-4. 95085100	0. 21321500
H	-3. 53962800	-5. 85941100	-0. 37145300
C	-4. 91226000	-4. 28100000	0. 22392800
H	-5. 73970500	-4. 67962900	-0. 35688700
C	-5. 07338300	-3. 14200300	0. 96487600

H	-6.02651400	-2.61902400	0.97875400
C	-2.59581600	-4.46188500	0.92981300
H	-1.64791800	-4.98730200	0.91398000
N	0.36751100	-1.07774700	-1.63143000
S	-1.08299200	-0.85270500	-2.19441400
O	-1.10744900	0.13918600	-3.28308700
O	-2.14573800	-0.69418500	-1.15700900
C	-1.51834200	-2.46100500	-3.04050000
F	-0.62091300	-2.72504700	-3.99808000
F	-2.72916000	-2.35350400	-3.60234000
F	-1.53202800	-3.46906300	-2.16690000
C	-4.89974400	2.21444200	-0.93353500
C	-4.10446500	2.06820000	-2.27450500
H	-4.73651100	2.45576200	-3.08451200
H	-3.94045700	1.00425400	-2.46328000
C	-2.77936700	2.76165500	-2.38295100
C	-3.95059400	1.86696000	0.27188500
H	-4.12804900	2.56007100	1.09573700
H	-4.16906700	0.85611700	0.62111900
N	-2.50440200	1.84541500	-0.01494100
C	-1.57716300	2.67623700	0.51705500
N	-0.37117400	2.15857400	0.77771900
C	0.80703900	2.85158000	1.17591800
C	1.32857900	3.92530900	0.45365800
C	1.48882600	2.35500500	2.29095800
C	2.51338700	4.52663500	0.87932200
C	2.67338900	2.96288300	2.70062200
H	1.08963800	1.49818400	2.82102900
C	3.18805800	4.05719600	2.00538700
H	4.10923900	4.52689900	2.32766800
C	3.43797800	2.40049200	3.87092700
C	3.04591100	5.71525600	0.12356900
F	2.62539700	1.75577400	4.73884500
F	4.37950400	1.51716300	3.47691200
F	4.07528300	3.37469600	4.55920400
F	2.47834400	6.86973900	0.53788900
F	4.38239700	5.85583500	0.27870900
F	2.80224700	5.61431700	-1.20416100
S	-1.95374600	4.36250200	0.68399200
H	0.82939200	4.27922200	-0.43873000
H	-0.25850300	1.11762000	0.81366000
H	-2.17998700	0.90547200	-0.29780300
C	-2.54646200	4.12647200	-2.29983100
H	-3.37936200	4.82085200	-2.40350500

H	-2.33505500	4.29541800	-0.94951900
H	-1.59343500	4.49456600	-2.67958100
C	-5.44451500	3.68494900	-0.79289500
H	-5.96852700	3.92699800	-1.72828200
H	-4.59791300	4.36836400	-0.70442900
C	-6.10638800	1.25082500	-0.94254200
C	-6.69556000	0.79437600	-2.13096100
C	-6.69851700	0.84386000	0.26685400
C	-7.81403600	-0.04190700	-2.11493300
H	-6.28472500	1.07490000	-3.09441900
C	-7.81850000	0.01234000	0.28745200
H	-6.29595300	1.19264400	1.21250500
C	-8.38164100	-0.43973500	-0.90637400
H	-8.23669300	-0.38341100	-3.05596700
H	-8.25216600	-0.27729900	1.24116100
H	-9.25153600	-1.09040900	-0.89360900
C	-6.37590600	3.94715400	0.36227800
C	-6.07063300	4.70235500	1.42039000
H	-5.09723000	5.17652000	1.52633000
H	-6.78724100	4.87920600	2.21834400
H	-7.36487500	3.49730900	0.30054200
H	-1.93685600	2.11077700	-2.61335600

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1 imaginary frequency

H = -5236.772441

G = -5236.967088

E(M06-2X-DCM) = -5237.612266

E(M06-2X-cyclohexane) = -5237.583121

O	0.27731800	-2.90252300	0.16663500
O	2.42540500	-1.48402200	-0.04483200
P	0.80013000	-1.37037400	-0.09179700
O	0.38721900	-0.43228700	1.00094400
C	1.39538400	-4.72997600	3.76519500
C	2.22959700	-4.77957300	2.65326800
C	1.82858400	-4.22006200	1.43044300
C	-0.25303800	-3.47337000	2.46622000
C	0.15609300	-4.09944400	3.65537600
C	3.09539000	-2.25359700	-0.99813000
C	3.15331600	-3.63808600	-0.84980100
C	3.65752800	-4.41393900	-1.90575800
C	4.21607900	-3.80913400	-3.02681300
C	4.27505700	-2.41608100	-3.08812700
C	3.70640600	-1.60754100	-2.09063600

H	-0.51023500	-4.06298400	4.51243800
H	4.74890600	-1.93137000	-3.93664700
C	2.85095200	-4.54049800	0.34499500
C	4.13399100	-4.72994300	1.22717800
H	4.56422300	-3.74380800	1.43664600
H	4.90080300	-5.32828500	0.72578300
H	4.43690100	-6.36802200	-1.36679500
H	3.06539100	-6.43656000	-2.46749000
C	0.61829400	-3.53341600	1.36190600
H	1.70224100	-5.16973500	4.71085500
H	4.61508800	-4.40841800	-3.84144700
C	3.62169800	-5.36003300	2.53938000
H	4.25219300	-5.11536700	3.40174600
H	3.59123000	-6.45680600	2.47156100
C	3.47886800	-5.88890300	-1.61279300
C	2.52498600	-5.87855400	-0.39667700
H	1.48488500	-5.84578200	-0.74070900
H	2.63676600	-6.75401900	0.25101600
C	3.80586400	-0.11767700	-2.18656900
C	3.17243900	0.57576600	-3.24714800
C	4.59913900	0.58978700	-1.24727600
C	2.34076800	-0.07452800	-4.21501400
C	3.34155000	2.00728500	-3.36500000
C	4.73418400	2.02416300	-1.36236400
C	1.75882200	0.62433800	-5.23931100
H	2.14320400	-1.13387700	-4.10791100
C	2.71924200	2.69800500	-4.45203200
C	4.10390700	2.69258000	-2.41556100
C	1.95781600	2.02779300	-5.37048600
H	1.11754500	0.10637400	-5.94652600
H	2.86945300	3.77258700	-4.53019700
H	4.20343100	3.77310100	-2.49391300
H	1.49145000	2.56316500	-6.19358400
C	-1.58043700	-2.78462900	2.41936100
C	-1.79431800	-1.61890000	3.19457100
C	-2.63697100	-3.33522900	1.65422000
C	-0.75313800	-0.98763000	3.95049700
C	-3.10455300	-1.00960800	3.22215400
C	-3.93563100	-2.70189600	1.67006500
C	-0.99082700	0.13737600	4.69727300
H	0.24544800	-1.40506100	3.90894800
C	-3.31415400	0.15715500	4.02473000
C	-4.13713800	-1.56695600	2.46162500
C	-2.29233700	0.71604900	4.74426100

H	-0.17712700	0.59819500	5.25165200
H	-4.31228600	0.58979300	4.05217500
H	-5.12511600	-1.11101600	2.48865300
H	-2.46651200	1.60171300	5.34967000
C	6.05329700	0.66094600	0.71900700
H	6.57282300	0.14363900	1.52103100
C	5.30552500	-0.05336400	-0.17985400
H	5.24792400	-1.13176100	-0.08832000
C	6.15988000	2.07650400	0.61478000
H	6.75419500	2.62628400	1.33974300
C	5.52271600	2.73405100	-0.40248500
H	5.59468200	3.81455700	-0.49628300
C	-3.52913600	-5.02780900	0.13514600
H	-3.38589200	-5.92791600	-0.45660300
C	-4.80027400	-4.38662100	0.13818200
H	-5.61207700	-4.79833200	-0.45542200
C	-4.99539000	-3.25880700	0.88801700
H	-5.96021800	-2.75751900	0.89688200
C	-2.48786700	-4.52206700	0.86778200
H	-1.52825100	-5.02588300	0.85729400
N	0.42195200	-1.05555000	-1.63305000
S	-1.02961300	-0.86123100	-2.20513900
O	-1.07092700	0.14196300	-3.28276000
O	-2.10364600	-0.74110800	-1.17412100
C	-1.41697600	-2.47049300	-3.07245800
F	-0.50690100	-2.69926200	-4.02725000
F	-2.62664300	-2.38845900	-3.64072400
F	-1.40911100	-3.48881700	-2.21078200
C	-4.93348300	2.12406300	-0.86927800
C	-4.16461400	2.00072900	-2.22939900
H	-4.81499700	2.40042900	-3.01873200
H	-4.00392900	0.93987600	-2.43777400
C	-2.83980800	2.69405500	-2.35084700
C	-3.95706300	1.74534800	0.30583100
H	-4.12925900	2.38707700	1.16971100
H	-4.15164900	0.71412200	0.60633100
N	-2.51390800	1.76982200	0.00675400
C	-1.61056200	2.62492000	0.54150600
N	-0.38956600	2.14237500	0.79645000
C	0.76776000	2.86775200	1.19770200
C	1.25973100	3.95649300	0.47729600
C	1.46159500	2.38879000	2.31292800
C	2.42774900	4.58896700	0.90416600
C	2.62846900	3.02863800	2.72464800

H	1. 08537100	1. 52083100	2. 84179100
C	3. 11385800	4. 13690900	2. 03048800
H	4. 02185800	4. 63095900	2. 35383000
C	3. 40628300	2. 48688500	3. 89604300
C	2. 93024000	5. 79087600	0. 14868000
F	2. 61033000	1. 81829800	4. 76098500
F	4. 37356300	1. 63124800	3. 50307000
F	4. 01400200	3. 47810600	4. 58667500
F	2. 33555600	6. 93090400	0. 56462300
F	4. 26317100	5. 96328100	0. 30237800
F	2. 68751100	5. 68470600	-1. 17872100
S	-2. 04367300	4. 29642400	0. 72086600
H	0. 75142200	4. 29745300	-0. 41507800
H	-0. 24772700	1. 10416200	0. 82668400
H	-2. 16400700	0. 84240100	-0. 28653500
C	-2. 60493900	4. 05861300	-2. 27189100
H	-3. 43491700	4. 75566300	-2. 38132900
H	-2. 40789600	4. 22928500	-0. 91516800
H	-1. 64918900	4. 42360800	-2. 64767900
C	-5. 49088200	3. 58712600	-0. 71498000
H	-6. 12504000	3. 78981000	-1. 58655800
H	-4. 64844000	4. 28296000	-0. 75611100
C	-6. 13542800	1. 15660300	-0. 86229700
C	-6. 71449500	0. 66198000	-2. 03994700
C	-6. 72922900	0. 78021400	0. 35509500
C	-7. 82537200	-0. 18393200	-2. 00484400
H	-6. 30201300	0. 91892900	-3. 00927700
C	-7. 83856100	-0. 06406600	0. 39549900
H	-6. 33351600	1. 15792500	1. 29222000
C	-8. 39255100	-0. 55452200	-0. 78747300
H	-8. 24127100	-0. 55542400	-2. 93752700
H	-8. 27329200	-0. 33109100	1. 35524500
H	-9. 25592200	-1. 21347200	-0. 75957900
C	-6. 26543400	3. 90656800	0. 53615900
C	-7. 55184700	4. 25688600	0. 56352200
H	-8. 15444700	4. 29531000	-0. 34157300
H	-8. 05300800	4. 51940600	1. 49128900
H	-5. 70570900	3. 89900200	1. 47195500
H	-1. 99805500	2. 04365400	-2. 58503200

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l imaginary frequency

H = -5236. 765448

G = -5236. 961812

E(M06-2X-DCM) = -5237.610838

E(M06-2X-cyclohexane) = -5237.580322

O	2.69666000	-1.66351500	-0.29255100
O	2.14757200	0.67070900	-1.26492600
P	1.51130100	-0.53928600	-0.35644100
O	1.17711600	0.08441200	0.96914500
C	6.33256500	-0.62228300	1.49527700
C	6.07916900	-0.30091300	0.16529100
C	4.89158100	-0.71661100	-0.45659600
C	4.15287600	-1.72689300	1.64323200
C	5.38594900	-1.35874300	2.20827900
C	2.52851000	0.44385500	-2.58663300
C	3.75740700	-0.15943100	-2.85208000
C	4.05911600	-0.53798100	-4.17028200
C	3.20877200	-0.20340200	-5.21841600
C	2.04648100	0.51735000	-4.94430100
C	1.66995100	0.84344600	-3.63099100
H	5.58732700	-1.64406100	3.23665600
H	1.39325800	0.81928500	-5.75766200
C	4.96315000	-0.43528900	-1.95457400
C	5.95405300	0.77905700	-1.95666200
H	5.38987000	1.69422800	-1.74000300
H	6.44670400	0.91532400	-2.92421700
H	6.16972200	-0.71531900	-4.64548500
H	5.27714400	-2.22071200	-4.83296400
C	3.91684900	-1.35899400	0.30410500
H	7.25861100	-0.31515200	1.97498300
H	3.44624900	-0.48837700	-6.24025500
C	6.93730600	0.48510400	-0.80266500
H	7.35121200	1.39640100	-0.35556800
H	7.79361700	-0.11007200	-1.14960100
C	5.35570400	-1.31724100	-4.21757300
C	5.61078300	-1.63310900	-2.72769800
H	5.08717900	-2.55468100	-2.44915000
H	6.67006500	-1.76370900	-2.48523200
C	0.41569800	1.62900100	-3.40294700
C	-0.84285300	1.07898900	-3.75169400
C	0.49788400	2.96064500	-2.92133400
C	-0.99781000	-0.26745800	-4.21327000
C	-2.03834200	1.88289600	-3.62145900
C	-0.70877500	3.74459500	-2.77420500
C	-2.22697100	-0.77069300	-4.54830900
H	-0.12618600	-0.90669600	-4.25746400
C	-3.30255100	1.32120700	-3.98866400

C	-1.94014300	3.18754100	-3.13145400
C	-3.39746300	0.03397400	-4.44729000
H	-2.31471100	-1.80441200	-4.86845600
H	-4.19168400	1.93964900	-3.88859800
H	-2.84287100	3.78736800	-3.03199400
H	-4.36501900	-0.38479100	-4.70677500
C	3.15750000	-2.50133400	2.44660400
C	2.59648200	-1.93373400	3.61762100
C	2.81724100	-3.82327300	2.06517700
C	2.89527000	-0.60499500	4.06344100
C	1.67408400	-2.70990300	4.41595500
C	1.87153500	-4.57459800	2.85760900
C	2.36661600	-0.10275100	5.22549200
H	3.55260300	0.01311700	3.46325800
C	1.13380400	-2.14346000	5.61317500
C	1.32890500	-4.00053900	4.00896700
C	1.47471800	-0.88086100	6.01811800
H	2.62964300	0.90246300	5.54548000
H	0.44787700	-2.74864200	6.20173900
H	0.62448000	-4.57539600	4.60677900
H	1.06923200	-0.46909200	6.93880400
C	1.78446700	4.88129700	-2.11762600
H	2.74132700	5.32962200	-1.86533600
C	1.73867900	3.59413300	-2.58719600
H	2.66054500	3.03917100	-2.71623200
C	0.59028200	5.63920500	-1.95496100
H	0.64535400	6.65870300	-1.58283600
C	-0.61817700	5.08409600	-2.27981600
H	-1.53796100	5.65423900	-2.17161000
C	3.03340500	-5.75483800	0.58340700
H	3.48385300	-6.22376600	-0.28735100
C	2.07957200	-6.47881700	1.35298600
H	1.80349300	-7.48774800	1.05892500
C	1.52143200	-5.90252400	2.46063700
H	0.79740500	-6.44454800	3.06421000
C	3.39068000	-4.47827600	0.92884400
H	4.12763500	-3.95080200	0.33460800
N	0.34020900	-1.19077000	-1.24640900
S	-0.59625600	-2.37790500	-0.75749400
O	-2.01461100	-1.99366600	-0.96391500
O	-0.24912300	-3.00045800	0.52765900
C	-0.28464800	-3.70530300	-2.03365000
F	-0.55003200	-3.26895400	-3.27349700
F	-1.07036500	-4.75574300	-1.77501700

F	0.99325200	-4.09150300	-1.98056000
C	0.26025000	3.51625600	2.39910900
C	0.39132400	2.34490500	3.44855000
H	0.71015700	2.80391000	4.39437500
H	1.19275000	1.68311200	3.11967000
C	-0.81469100	1.49930900	3.70874600
C	-0.42139100	2.98690000	1.08254800
H	-1.15617000	3.71594700	0.74237500
H	0.32033900	2.87523900	0.29204300
N	-1.09014200	1.67022200	1.17406600
C	-2.41659200	1.45849700	1.02759000
N	-2.82848300	0.30386300	0.47666400
C	-4.18073400	-0.15651800	0.40533300
C	-4.92088700	-0.42776100	1.55789600
C	-4.72552600	-0.39601800	-0.85403000
C	-6.22312900	-0.90703400	1.44061900
C	-6.03130400	-0.88231700	-0.95776000
H	-4.13232500	-0.20999100	-1.74281500
C	-6.78780500	-1.13518600	0.18288800
H	-7.79828200	-1.51559100	0.09751800
C	-6.60086300	-1.11616900	-2.33355900
C	-7.04890100	-1.13626200	2.67935800
F	-5.88717600	-2.03393800	-3.01995300
F	-7.87957600	-1.54259600	-2.29136000
F	-6.57844000	0.02124900	-3.07167800
F	-7.78083000	-0.04334900	2.99617500
F	-7.91630500	-2.15782800	2.51994000
F	-6.27679100	-1.41703300	3.75253500
S	-3.53663000	2.59992600	1.69963900
H	-4.48213500	-0.27598300	2.53585900
H	-2.18107900	-0.28823900	-0.06363500
H	-0.43087100	0.89215000	0.97710800
C	-2.02083800	1.92228600	4.25611400
H	-2.04613200	2.86643500	4.79979700
H	-2.71142100	2.30920900	3.16047700
H	-2.69307500	1.15666100	4.64372900
C	-0.61365000	4.67280800	2.97703400
H	-0.17703100	4.99627300	3.93222600
H	-1.60677200	4.28531100	3.21052400
C	1.71713800	3.97375100	2.13806300
C	2.26003600	5.13099500	2.71773100
C	2.58114600	3.15897700	1.38573500
C	3.60022600	5.47854000	2.52929100
H	1.64871000	5.78542500	3.32868100

C	3.91997500	3.50137400	1.20141600
H	2.22339300	2.22796500	0.95872000
C	4.43751300	4.66790000	1.76592700
H	3.98469200	6.38615000	2.98744300
H	4.55818000	2.84026600	0.62128600
H	5.48057500	4.93634100	1.62083500
C	-0.79144300	5.86428600	2.06649800
C	-1.97429100	6.39084100	1.74341400
H	-2.05094600	7.26350400	1.10009200
H	-2.91034400	5.97348900	2.10788800
H	0.11250700	6.31446200	1.66125500
H	-0.70749900	0.44247700	3.47312000

TS-EF-3RS-6

1 imaginary frequency

H = -5236.762942

G = -5236.961433

E(M06-2X-DCM) = -5237.606744

E(M06-2X-cyclohexane) = -5237.576058

O	2.55649500	-1.64094400	-0.74059400
O	2.27568600	0.92137200	-1.04404600
P	1.50727100	-0.41396800	-0.47995800
O	1.20174500	-0.15351300	0.96529000
C	6.28701300	-1.55785200	1.15114700
C	6.07257700	-0.85196700	-0.02831700
C	4.84557200	-0.94521200	-0.70159400
C	3.99167200	-2.40707800	1.05951800
C	5.26089400	-2.35330200	1.66177500
C	2.64146000	1.00663600	-2.38691900
C	3.79002300	0.35208300	-2.83272500
C	4.05016500	0.29718200	-4.21216300
C	3.24879900	0.98389500	-5.11718900
C	2.18406400	1.74490400	-4.63520100
C	1.85053800	1.76812200	-3.27166800
H	5.42886900	-2.93731100	2.56190100
H	1.57697100	2.32481000	-5.32430000
C	4.95291800	-0.28216800	-2.07039700
C	6.07289500	0.77292300	-1.77390700
H	5.61308100	1.64912700	-1.30222000
H	6.58068400	1.11058900	-2.68270300
H	6.12760300	0.02125900	-4.77310300
H	5.07285600	-1.27685300	-5.32197200
C	3.80022900	-1.65522000	-0.11647300
H	7.24248600	-1.50287200	1.66699400

H	3.45330800	0.94339700	-6.18408600
C	7.01396800	0.07386200	-0.76796900
H	7.51813900	0.78132200	-0.09950200
H	7.80459400	-0.48919900	-1.28359600
C	5.25042600	-0.57987300	-4.49499100
C	5.46432600	-1.29873400	-3.14611600
H	4.83937100	-2.19803800	-3.10280900
H	6.50134500	-1.60326500	-2.97381300
C	0.72868900	2.64961300	-2.81484200
C	-0.60748100	2.36597100	-3.18691300
C	1.02928600	3.84100600	-2.10685800
C	-0.97227700	1.18668800	-3.91148900
C	-1.66353100	3.28625300	-2.82581400
C	-0.03900200	4.74176800	-1.73376800
C	-2.27077900	0.94702400	-4.27614800
H	-0.20546300	0.45985400	-4.14227500
C	-3.00613000	3.00082800	-3.22951200
C	-1.35406800	4.43800300	-2.09781400
C	-3.30415600	1.87010100	-3.94321900
H	-2.51980500	0.03030400	-4.80183300
H	-3.78671100	3.70835900	-2.95899400
H	-2.15237400	5.12677500	-1.82778000
H	-4.32856000	1.66245800	-4.23909700
C	2.91717300	-3.26085900	1.65254100
C	2.44924600	-2.99966500	2.96505600
C	2.41112600	-4.36829600	0.92675100
C	2.91788800	-1.90222600	3.75877800
C	1.45195600	-3.86566300	3.55391600
C	1.39153600	-5.20452000	1.51697000
C	2.47951700	-1.70775200	5.04402600
H	3.63281400	-1.21203000	3.32682100
C	1.00937800	-3.61794200	4.89152300
C	0.94236600	-4.93312300	2.81089800
C	1.51369800	-2.57792600	5.62569300
H	2.87012600	-0.87556000	5.62471000
H	0.26550200	-4.28786500	5.31713800
H	0.18342100	-5.57468300	3.25436000
H	1.18103200	-2.41254400	6.64728800
C	2.63018000	5.40919600	-1.12565100
H	3.65864700	5.68837600	-0.91155800
C	2.36740400	4.23209800	-1.77766900
H	3.18736300	3.58700300	-2.07151800
C	1.57111300	6.27815100	-0.73497300
H	1.79688900	7.20573900	-0.21565700

C	0.27554200	5.94711400	-1.03013800
H	-0.54256000	6.60745300	-0.75162700
C	2.36733100	-5.79989500	-1.05350900
H	2.74458600	-6.04475700	-2.04277000
C	1.34119500	-6.60101500	-0.47789800
H	0.93811700	-7.44262300	-1.03455200
C	0.87405900	-6.31094800	0.77423100
H	0.09734400	-6.91853700	1.23239800
C	2.88431000	-4.72793900	-0.37541000
H	3.67341700	-4.13979200	-0.82869200
N	0.28345500	-0.67449000	-1.49913400
S	-0.68799200	-1.92698500	-1.44380200
O	-2.08736200	-1.45488800	-1.59423400
O	-0.42563700	-2.91921700	-0.39176700
C	-0.33836100	-2.81633000	-3.04860000
F	-0.58202200	-2.02569800	-4.10588100
F	-1.12127700	-3.89607500	-3.13779700
F	0.94130000	-3.19958100	-3.08773600
C	0.26968600	2.45214400	3.44227900
C	0.36445300	0.97364900	3.95675500
H	0.66908000	0.99519500	5.00937300
H	1.15059500	0.47082900	3.39120800
C	-0.87375700	0.13526500	3.88428900
C	-0.34950900	2.44317600	2.00029500
H	-0.99269500	3.31315100	1.86164100
H	0.45505300	2.48050000	1.26632200
N	-1.10453800	1.22918300	1.61544200
C	-2.43392400	1.14566900	1.40467200
N	-2.88699700	0.27928600	0.48342300
C	-4.24663700	-0.10313300	0.26529700
C	-5.02265900	-0.67708400	1.27510400
C	-4.76241900	0.04193600	-1.02062700
C	-6.32999500	-1.06779700	0.99768900
C	-6.07270400	-0.36197600	-1.28763700
H	-4.14186400	0.46204600	-1.80420600
C	-6.86564100	-0.90944000	-0.28344600
H	-7.88462400	-1.21193400	-0.49228300
C	-6.61641400	-0.15372900	-2.67782200
C	-7.15755100	-1.73235000	2.06705700
F	-5.79700200	-0.67698200	-3.61479300
F	-7.83345600	-0.71073200	-2.83933700
F	-6.73604600	1.16627500	-2.96492500
F	-7.09762700	-3.07953600	1.97761900
F	-6.73747700	-1.39898200	3.30784200

F	-8.46029100	-1.38925200	1.97078100
S	-3.50832300	2.02420100	2.44735900
H	-4.61316900	-0.81666800	2.26698800
H	-2.25159700	-0.11936500	-0.22416500
H	-0.47277600	0.54382200	1.16063300
C	-2.06316800	0.36720300	4.55891300
H	-2.06513900	1.05405300	5.40453200
H	-2.74232400	1.18549200	3.67202500
H	-2.77399000	-0.45533700	4.63470400
C	-0.59808900	3.33278900	4.41255200
H	-0.19556600	3.19006800	5.42569600
H	-1.62869600	2.97369100	4.41598100
C	1.69425400	3.05358700	3.43340500
C	2.12130400	3.94703600	2.43844100
C	2.58609300	2.79166500	4.48762200
C	3.39004100	4.52839800	2.48247400
H	1.46943400	4.22039100	1.61614200
C	3.85432500	3.36977500	4.53372400
H	2.30187100	2.12526000	5.29560600
C	4.26680800	4.24086500	3.52609900
H	3.68478600	5.20763200	1.68813200
H	4.51892100	3.13476000	5.36101800
H	5.25533300	4.69089400	3.55703800
C	-0.61151700	4.80710200	4.10104600
C	-1.69714300	5.49283200	3.73645300
H	-1.65484200	6.56123300	3.54096600
H	-2.66796300	5.01552100	3.62292100
H	0.33809500	5.32994700	4.19841500
H	-0.79832100	-0.76627600	3.27973000

TS-EF-3RS-7

l imaginary frequency

H = -5236.766094

G = -5236.962231

E(M06-2X-DCM) = -5237.609670

E(M06-2X-cyclohexane) = -5237.578949

O	2.70205200	-1.08720200	1.28358900
O	2.12749500	-0.91507300	-1.23839900
P	1.51945100	-0.61744800	0.25568200
O	1.20642200	0.84889900	0.29923200
C	6.36701400	0.92682000	1.16851100
C	6.08770000	-0.09067600	0.26186200
C	4.89381600	-0.82154300	0.35577800
C	4.19226700	0.57163600	2.23676000

C	5.43682900	1.22137400	2.16597800
C	2.49936400	-2.20395100	-1.61508400
C	3.73589400	-2.70786200	-1.21029000
C	4.03635000	-4.05690600	-1.46086700
C	3.17342600	-4.85352700	-2.20496300
C	1.99952800	-4.29305700	-2.70701100
C	1.62842800	-2.96998100	-2.41719300
H	5.66014400	1.98850400	2.90164600
H	1.33427800	-4.89157300	-3.32246400
C	4.94977600	-2.02408700	-0.58129000
C	5.91916900	-1.46743200	-1.67877400
H	5.34180000	-0.84995300	-2.37655300
H	6.39983600	-2.26366400	-2.25563900
H	6.14700300	-4.54809500	-1.56301300
H	5.28863700	-5.39768500	-0.28227100
C	3.93135100	-0.43472400	1.28520100
H	7.30047100	1.48154700	1.11236800
H	3.41041300	-5.89565800	-2.40388500
C	6.91964900	-0.58146900	-0.90347900
H	7.31458400	0.24055800	-1.51167500
H	7.78694900	-1.16244400	-0.55970800
C	5.34912100	-4.44152500	-0.81454300
C	5.61704200	-3.25042300	0.12907600
H	5.11257800	-3.41694000	1.08772700
H	6.67947100	-3.08703300	0.33459900
C	0.36580400	-2.42658700	-3.01263200
C	-0.89013000	-2.96009500	-2.63258500
C	0.43962100	-1.45661100	-4.04423200
C	-1.03198500	-3.94129000	-1.59974400
C	-2.09356300	-2.50380500	-3.29298000
C	-0.77383500	-0.99256100	-4.67999200
C	-2.25721600	-4.45563100	-1.26777500
H	-0.15249200	-4.25055500	-1.05092500
C	-3.35404500	-3.06786200	-2.91693200
C	-2.00483100	-1.52490800	-4.28590300
C	-3.43611100	-4.02457300	-1.94001400
H	-2.33535200	-5.18029500	-0.46322700
H	-4.25014800	-2.71731100	-3.42395100
H	-2.91326600	-1.18417800	-4.77914700
H	-4.40020400	-4.43570500	-1.65668000
C	3.21190600	0.93816300	3.30448000
C	2.69725600	2.25754900	3.37212500
C	2.83838200	-0.01862200	4.28178700
C	3.03928300	3.28136300	2.42919900

C	1. 78281800	2. 61453400	4. 43387000
C	1. 89981400	0. 34568300	5. 31770800
C	2. 55950400	4. 56068800	2. 55325700
H	3. 69245500	3. 03113700	1. 60150700
C	1. 29070400	3. 95517300	4. 51599400
C	1. 39916900	1. 64811600	5. 36606900
C	1. 67286800	4. 90929400	3. 61185800
H	2. 85824800	5. 32124400	1. 83536000
H	0. 60843300	4. 20113000	5. 32662400
H	0. 69984000	1. 91871400	6. 15456900
H	1. 30426000	5. 92831300	3. 69605800
C	1. 72255500	-0. 02003300	-5. 55252100
H	2. 68185000	0. 34594600	-5. 90789900
C	1. 68087100	-0. 93365400	-4. 53154400
H	2. 60574100	-1. 28545800	-4. 08931000
C	0. 52256200	0. 45140100	-6. 15802300
H	0. 57376500	1. 17245500	-6. 96993700
C	-0. 68839700	-0. 02197200	-5. 72773400
H	-1. 61267500	0. 31509900	-6. 19172300
C	2. 98415500	-2. 24949600	5. 26989900
H	3. 40577700	-3. 25109100	5. 26715900
C	2. 03490600	-1. 89269600	6. 26872200
H	1. 73289600	-2. 62548800	7. 01199900
C	1. 51464200	-0. 62805100	6. 29085100
H	0. 79565100	-0. 33589100	7. 05242500
C	3. 37280300	-1. 34613600	4. 31620600
H	4. 10578900	-1. 63681600	3. 57291700
N	0. 33071900	-1. 68720900	0. 46123500
S	-0. 62454700	-1. 72035300	1. 72721000
O	-2. 03897400	-1. 74743700	1. 27189800
O	-0. 29769500	-0. 79976100	2. 82583800
C	-0. 33788800	-3. 42775200	2. 42762700
F	-0. 59362200	-4. 38164100	1. 52029600
F	-1. 14339500	-3. 61331700	3. 47855500
F	0. 93236900	-3. 54506600	2. 82391900
C	0. 31913500	3. 71706600	-1. 85118500
C	0. 40949000	3. 99621800	-0. 31929300
H	0. 75806100	5. 02935200	-0. 18781100
H	1. 15533600	3. 32499900	0. 10856700
C	-0. 84655400	3. 84866100	0. 47828300
C	-0. 33646800	2. 30029400	-2. 08278200
H	-1. 00066400	2. 32821100	-2. 94755700
H	0. 45508300	1. 57432400	-2. 27453000
N	-1. 08758400	1. 73390500	-0. 94446100

C	-2.42012300	1.54340900	-0.88120000
N	-2.89136500	0.53111100	-0.13424600
C	-4.25835800	0.29308300	0.20706900
C	-5.01713800	1.23564600	0.90525200
C	-4.80199900	-0.94950700	-0.11189400
C	-6.33438800	0.94050800	1.24674700
C	-6.12347900	-1.23463400	0.24141700
H	-4.19553500	-1.68718500	-0.62630500
C	-6.89782400	-0.29445800	0.91485000
H	-7.92061300	-0.52136900	1.18954900
C	-6.69090200	-2.57955700	-0.13422400
C	-7.17689300	1.97926700	1.93992100
F	-6.00430000	-3.58952200	0.44181400
F	-7.98367200	-2.70769600	0.22715800
F	-6.62401300	-2.78175100	-1.47362200
F	-7.88241300	2.71757200	1.05278400
F	-8.06946300	1.41745700	2.78207200
F	-6.42210800	2.84099500	2.65724800
S	-3.47400200	2.70786500	-1.62472700
H	-4.58246900	2.18543800	1.18838300
H	-2.26944400	-0.23148900	0.18036800
H	-0.45661900	1.18081300	-0.33389300
C	-2.01854400	4.56886900	0.30671000
H	-1.98027400	5.49581500	-0.26411000
H	-2.69210500	3.80672800	-0.62638700
H	-2.74588400	4.55336900	1.11837300
C	-0.51768400	4.80209400	-2.61126600
H	-1.57664400	4.71750100	-2.35693200
H	-0.45168700	4.55446000	-3.67989600
C	1.73439200	3.71910900	-2.47031000
C	1.89923300	3.29053300	-3.79877300
C	2.87344700	4.17302000	-1.79058200
C	3.14618800	3.31613100	-4.42049400
H	1.04758300	2.91877500	-4.36205100
C	4.12469300	4.20180600	-2.41193000
H	2.80567500	4.50532100	-0.76112600
C	4.26823200	3.77630900	-3.73040600
H	3.23781700	2.97526900	-5.44813700
H	4.98733700	4.55807000	-1.85517200
H	5.24084200	3.80009100	-4.21422500
C	-0.04989000	6.21971200	-2.42108900
C	-0.84670000	7.25691300	-2.15275800
H	-0.45711200	8.26663800	-2.05523600
H	-1.92441200	7.14427200	-2.04498700

H	1.01925500	6.39261900	-2.54370300
H	-0.80374800	3.13062500	1.29529000

TS-EF-3RS-8

l imaginary frequency

H = -5236.763387

G = -5236.959973

E(M06-2X-DCM) = -5237.608586

E(M06-2X-cyclohexane) = -5237.576641

O	2.65623900	-1.35273100	1.09371700
O	2.08185800	-0.73964300	-1.35897100
P	1.48153900	-0.69317300	0.16645900
O	1.19632500	0.74965200	0.46284800
C	6.35508400	0.58882800	1.31318900
C	6.05717500	-0.25159900	0.24537900
C	4.85114400	-0.96788100	0.21672400
C	4.17596300	0.09059600	2.31327400
C	5.43154100	0.72172500	2.35067000
C	2.43112100	-1.95047700	-1.95343200
C	3.65940800	-2.53681000	-1.64625600
C	3.93676500	-3.82728900	-2.12657800
C	3.05944400	-4.46969700	-2.99291900
C	1.89476600	-3.81179900	-3.38655900
C	1.54662600	-2.55216300	-2.87234900
H	5.66929600	1.34592600	3.20705400
H	1.21907700	-4.28428400	-4.09350700
C	4.88550100	-1.99126400	-0.91418500
C	5.86200300	-1.26881400	-1.90335000
H	5.29389200	-0.53027900	-2.48069800
H	6.32792000	-1.96088400	-2.61171700
H	6.03867100	-4.32730100	-2.32169200
H	5.16879800	-5.37100700	-1.20230500
C	3.89673000	-0.73133900	1.20296500
H	7.29776900	1.12937700	1.34979300
H	3.27849000	-5.46580900	-3.36915300
C	6.87878000	-0.54708600	-0.99100400
H	7.28667500	0.36114000	-1.44958500
H	7.73647200	-1.19316600	-0.75674700
C	5.24412000	-4.33854900	-1.56226300
C	5.53364700	-3.33222300	-0.42895600
H	5.02835200	-3.65334300	0.48909000
H	6.59902700	-3.22367900	-0.20342500
C	0.29432800	-1.89225900	-3.36268700
C	-0.97150000	-2.45992700	-3.07671000

C	0.38680000	-0.76148300	-4.21324800
C	-1.13230400	-3.60102900	-2.22721800
C	-2.16582300	-1.87522000	-3.64622400
C	-0.81748000	-0.17273200	-4.75646100
C	-2.36711300	-4.14217500	-1.98555700
H	-0.25896400	-4.01626000	-1.74217000
C	-3.43678600	-2.47226300	-3.36958400
C	-2.05836100	-0.74214200	-4.45648100
C	-3.53727000	-3.58064200	-2.57098800
H	-2.45932700	-4.99284800	-1.31745100
H	-4.32595900	-2.02349000	-3.80647800
H	-2.96001900	-0.30508700	-4.88149400
H	-4.50907800	-4.01618500	-2.35974200
C	3.20330700	0.28271800	3.43248900
C	2.71454400	1.57938600	3.73300300
C	2.81162600	-0.82343900	4.22828100
C	3.07527500	2.74622600	2.98294200
C	1.80872600	1.76189200	4.84532400
C	1.88083800	-0.62883500	5.31577000
C	2.62179800	3.99301700	3.33262000
H	3.72189100	2.63312800	2.12073500
C	1.34419100	3.07655700	5.16473800
C	1.40648400	0.65428900	5.59468200
C	1.74453100	4.16732100	4.44091800
H	2.93563800	4.86182100	2.75832400
H	0.66857900	3.18931300	6.00969500
H	0.71341600	0.79560100	6.42154200
H	1.39762100	5.16276000	4.70593700
C	1.69699200	0.88821200	-5.45680900
H	2.66312100	1.29160700	-5.74714600
C	1.63785100	-0.18618000	-4.60766500
H	2.55587400	-0.62596400	-4.23548400
C	0.50627500	1.47933600	-5.96820800
H	0.57134400	2.32839300	-6.64391200
C	-0.71349700	0.96173000	-5.62203500
H	-1.63115200	1.39093800	-6.01809300
C	2.91352600	-3.19564800	4.80867700
H	3.31553700	-4.18909500	4.62863500
C	1.97142800	-3.00176200	5.85790800
H	1.65496000	-3.84786200	6.46173900
C	1.47650300	-1.75079500	6.10400100
H	0.76361600	-1.58303400	6.90770400
C	3.32003300	-2.14642900	4.02734200
H	4.04759700	-2.31613000	3.24245900

N	0.27453400	-1.76110100	0.19162300
S	-0.69348600	-1.97560800	1.42997100
O	-2.10416800	-1.88217300	0.97162800
O	-0.34970100	-1.26326700	2.66925400
C	-0.46204500	-3.78414700	1.83389400
F	-0.73402000	-4.56380900	0.77735800
F	-1.28401100	-4.12007700	2.83357600
F	0.80000100	-4.00333000	2.21279700
C	0.42064500	3.96959700	-1.17202700
C	0.50598300	3.95713400	0.38458500
H	0.91526900	4.92053900	0.71468200
H	1.20997600	3.17812900	0.68111900
C	-0.76779600	3.73140900	1.13525600
C	-0.28158900	2.63774100	-1.64748800
H	-0.94420200	2.83834300	-2.49027800
H	0.48573300	1.93075900	-1.96658900
N	-1.05285100	1.90789800	-0.62001200
C	-2.39045600	1.73664600	-0.59730500
N	-2.88776000	0.62360800	-0.03274300
C	-4.26277800	0.36350800	0.25767900
C	-5.00307200	1.18984600	1.10654600
C	-4.83451500	-0.79059500	-0.27361900
C	-6.32958100	0.87382500	1.38817600
C	-6.16513700	-1.09883100	0.02131900
H	-4.24292000	-1.44311200	-0.90661300
C	-6.92079200	-0.27015700	0.84557900
H	-7.95081400	-0.51495600	1.07391000
C	-6.76304200	-2.34396200	-0.58219600
C	-7.15085300	1.79835900	2.24845600
F	-6.11060800	-3.45598300	-0.18085700
F	-8.06310800	-2.49520400	-0.25771100
F	-6.68513900	-2.31762500	-1.93585800
F	-7.82593500	2.70143600	1.50117100
F	-8.06754200	1.12333900	2.97331800
F	-6.38027900	2.49824800	3.11068600
S	-3.41341100	3.03133300	-1.13865500
H	-4.54711100	2.06487600	1.55118700
H	-2.28513300	-0.19484700	0.15272300
H	-0.43905200	1.24136600	-0.11292000
C	-1.92052000	4.50380200	1.07473500
H	-1.86439600	5.50844400	0.65740800
H	-2.60938700	3.92744800	0.04264200
H	-2.64807800	4.38477100	1.87758900
C	-0.37876400	5.19877600	-1.73351500

H	-1.44071700	5.07058500	-1.50167900
H	-0.30891200	5.16047900	-2.82608000
C	1.83779000	4.03606500	-1.77785800
C	2.00103600	3.82308800	-3.15702500
C	2.98117300	4.34828700	-1.03109100
C	3.25225800	3.91972800	-3.76339600
H	1.14430600	3.56827100	-3.77516000
C	4.23692800	4.44546400	-1.63513400
H	2.91393000	4.51605600	0.03761000
C	4.37994900	4.23472600	-3.00453700
H	3.34294200	3.74745800	-4.83249100
H	5.10361100	4.68749400	-1.02569700
H	5.35629600	4.31263900	-3.47509800
C	0.08649500	6.55122100	-1.26414600
C	0.68554900	7.46170400	-2.03266800
H	0.98856900	8.42955700	-1.64238400
H	0.89840500	7.27222300	-3.08236600
H	-0.09775000	6.79935900	-0.21733200
H	-0.75815900	2.89459700	1.83142000

TS-EF-3RR

l imaginary frequency

H = -5236.781144

G = -5236.974114

E(M06-2X-DCM) = -5237.617532

E(M06-2X-cyclohexane) = -5237.589221

O	0.95827700	-2.79867100	0.17653400
O	2.72536200	-0.95103800	-0.18361100
P	1.11635900	-1.18938100	-0.09957800
O	0.59146700	-0.35591200	1.02763000
C	2.74641900	-4.33313100	3.63945600
C	3.47347400	-4.20508400	2.46067000
C	2.85905300	-3.74789900	1.28481900
C	0.76213800	-3.46285700	2.50379900
C	1.39657100	-3.98319000	3.64435200
C	3.46246200	-1.55675100	-1.20367100
C	3.83178900	-2.89484100	-1.08545800
C	4.40255700	-3.54237200	-2.19276200
C	4.72005200	-2.83042700	-3.34471700
C	4.46690800	-1.45838900	-3.38676700
C	3.82059700	-0.79357400	-2.33219400
H	0.81411200	-4.08716700	4.55524400
H	4.74957800	-0.88261000	-4.26314600
C	3.83229100	-3.84072200	0.11362900

C	5. 19522200	-3. 74631700	0. 88426400
H	5. 41775700	-2. 69011700	1. 07481100
H	6. 02851500	-4. 16428400	0. 31130000
H	5. 62972800	-5. 27929900	-1. 75224400
H	4. 22011200	-5. 64597600	-2. 74002300
C	1. 52770300	-3. 33794800	1. 32890100
H	3. 22024600	-4. 69381800	4. 54894700
H	5. 17105500	-3. 32825300	-4. 19957300
C	4. 94314300	-4. 47131500	2. 22270100
H	5. 57613000	-4. 09545300	3. 03453800
H	5. 14401800	-5. 54881300	2. 13866500
C	4. 57356400	-5. 02066900	-1. 91208500
C	3. 74376400	-5. 21791000	-0. 62296400
H	2. 69652100	-5. 41224200	-0. 88144200
H	4. 09577300	-6. 04808400	-0. 00220400
C	3. 57210500	0. 67944600	-2. 40776700
C	2. 71168900	1. 21128900	-3. 39948600
C	4. 25107300	1. 54713400	-1. 51446100
C	1. 97998400	0. 39087000	-4. 31775300
C	2. 53092900	2. 64305700	-3. 49246100
C	4. 03119800	2. 97290600	-1. 59745800
C	1. 17184300	0. 94071300	-5. 27739200
H	2. 04419500	-0. 68603900	-4. 22321700
C	1. 68130300	3. 17598300	-4. 51243600
C	3. 17960800	3. 48136400	-2. 58219700
C	1. 02727300	2. 35267000	-5. 38809800
H	0. 61618500	0. 29163900	-5. 94814400
H	1. 57014000	4. 25638100	-4. 57451900
H	3. 01365100	4. 55484100	-2. 63582000
H	0. 38621400	2. 76962700	-6. 16066600
C	-0. 68192900	-3. 07862800	2. 58998500
C	-1. 06836100	-1. 98685100	3. 40505700
C	-1. 66354000	-3. 85459200	1. 92720100
C	-0. 12021100	-1. 13193500	4. 05616800
C	-2. 47142100	-1. 68990300	3. 58558200
C	-3. 06280000	-3. 53938700	2. 10478700
C	-0. 52274400	-0. 08300700	4. 84170100
H	0. 93612000	-1. 31275700	3. 89958500
C	-2. 85014000	-0. 59416100	4. 42534400
C	-3. 42820300	-2. 47642200	2. 93667200
C	-1. 90804600	0. 18722900	5. 03811000
H	0. 22145600	0. 55738000	5. 30795500
H	-3. 91074400	-0. 39595400	4. 56571200
H	-4. 48493900	-2. 26345800	3. 09138100

H	-2.21031400	1.01775800	5.67043800
C	5.80365200	1.94438300	0.33370600
H	6.49699300	1.55865500	1.07621800
C	5.17658000	1.08096900	-0.52551100
H	5.38673000	0.01950700	-0.46313100
C	5.55776800	3.34475600	0.26649600
H	6.05923900	4.01289000	0.96156800
C	4.70014000	3.84100500	-0.67735800
H	4.50211700	4.90706300	-0.74439800
C	-2.30889900	-5.70613900	0.46859400
H	-2.03014800	-6.54562800	-0.16251700
C	-3.68525000	-5.38415200	0.63822600
H	-4.44370200	-5.97793600	0.13531100
C	-4.04721900	-4.33434100	1.43834900
H	-5.09587200	-4.08534200	1.58447200
C	-1.33599300	-4.97210100	1.09460400
H	-0.29355700	-5.23700400	0.96121600
N	0.55788900	-0.97230000	-1.60529500
S	-0.94206400	-1.12369200	-2.04106400
O	-1.33872800	-0.13747100	-3.05983200
O	-1.90789600	-1.30681800	-0.91449400
C	-1.00318900	-2.76026500	-2.94215400
F	-0.15385500	-2.74526300	-3.97532600
F	-2.24456500	-2.96601000	-3.41404000
F	-0.68127700	-3.76427100	-2.12573100
C	-5.19322600	0.40566500	-0.60092200
C	-4.43848900	0.70167300	-1.92889000
H	-5.14456100	0.63716500	-2.76937100
H	-3.72353300	-0.10265000	-2.10148600
C	-3.69909600	1.98615300	-2.04937400
C	-4.28560200	0.82381300	0.61872600
H	-4.67233700	1.72601400	1.08865100
H	-4.29418500	0.02134400	1.36537500
N	-2.87985900	1.08458400	0.28786400
C	-2.16538300	2.13457600	0.77208300
N	-0.84053100	1.95649100	0.89001500
C	0.13413400	2.93141500	1.24416400
C	0.24452800	4.15830100	0.58531600
C	1.04202000	2.59066100	2.25040400
C	1.23873600	5.05644400	0.97037800
C	2.03460300	3.49732100	2.62057300
H	0.96220100	1.62448900	2.73438900
C	2.13414600	4.73744900	1.99245500
H	2.89287300	5.44778000	2.29843900

C	3.02857500	3.11512100	3.68678400
C	1.38732500	6.36640300	0.24273100
F	2.48519300	2.27722600	4.60040200
F	4.10640300	2.48885500	3.16960000
F	3.48377700	4.19983700	4.35347300
F	1.77148900	7.35790500	1.07451900
F	2.32846600	6.29812800	-0.73584700
F	0.23857600	6.75073500	-0.35168800
S	-2.95753800	3.63599300	1.10744500
H	-0.43925600	4.41448200	-0.21229800
H	-0.45341400	0.98701900	0.87783200
H	-2.35156900	0.24918500	-0.00969800
C	-4.14519800	3.26445900	-1.69852800
H	-5.21250000	3.40539400	-1.52608900
H	-3.69964900	3.43493100	-0.50990500
H	-3.64475700	4.10081400	-2.18979300
C	-5.40066700	-1.15161900	-0.54267700
H	-5.90495400	-1.37678400	0.40762700
H	-4.41460900	-1.62759900	-0.50778800
C	-6.56784200	1.08773500	-0.46626700
C	-7.21353300	1.08134200	0.78380700
C	-7.25732600	1.66834000	-1.54076300
C	-8.47712700	1.64312300	0.95665500
H	-6.72583400	0.62696300	1.64220500
C	-8.52491900	2.23342000	-1.37296900
H	-6.81525900	1.69079800	-2.53150600
C	-9.14114500	2.22625400	-0.12370300
H	-8.94262600	1.62340400	1.93838400
H	-9.02716700	2.67845200	-2.22780500
H	-10.12566600	2.66618500	0.00746100
C	-6.20391000	-1.72650300	-1.67689800
C	-5.71660000	-2.57393100	-2.58601700
H	-4.67964100	-2.90063500	-2.56668200
H	-6.33930300	-2.97160100	-3.38359200
H	-2.70602200	1.89159200	-2.49031900
H	-7.24898700	-1.42143300	-1.73548900

TS-EF-3RR-1

1 imaginary frequency

H = -5236.777706

G = -5236.972031

E(M06-2X-DCM) = -5237.611300

E(M06-2X-cyclohexane) = -5237.583570

O	1.57904500	-2.64383100	-0.21451400
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O	2.59244600	-0.29323200	-0.59418300
P	1.16944100	-1.06766400	-0.38415200
O	0.52189400	-0.49802300	0.83913500
C	4.38698200	-3.73456600	2.69535100
C	4.79547400	-3.31706100	1.43309700
C	3.85438400	-2.99662300	0.44273300
C	2.05077100	-3.46231500	2.02315400
C	3.02303600	-3.82214200	2.97122500
C	3.31799300	-0.51624200	-1.76630200
C	4.05841100	-1.68648900	-1.90895000
C	4.57631900	-2.01258600	-3.17211100
C	4.47875300	-1.11442000	-4.23015800
C	3.87902900	0.12861500	-4.01347100
C	3.27875200	0.45322000	-2.78698900
H	2.68869100	-4.15919000	3.94817600
H	3.85258100	0.86381700	-4.81266100
C	4.55774000	-2.69538100	-0.87756100
C	5.96446500	-2.25079200	-0.34070700
H	5.91149200	-1.19376700	-0.05535500
H	6.75011300	-2.35291700	-1.09542500
H	6.28877100	-3.34901000	-3.20214300
H	4.86353600	-4.01338800	-3.99176700
C	2.49742300	-3.02879000	0.76034300
H	5.11658100	-3.98622900	3.46092500
H	4.88258300	-1.36132400	-5.20887200
C	6.20149500	-3.11138000	0.91660800
H	6.85369100	-2.62224400	1.64898600
H	6.67495500	-4.07038200	0.66213000
C	5.19224400	-3.39686400	-3.14721300
C	4.71923700	-3.95813200	-1.78479400
H	3.74064300	-4.43810700	-1.89904700
H	5.40707800	-4.69510900	-1.35772400
C	2.70346300	1.81666900	-2.55710700
C	1.54567900	2.24818900	-3.24830000
C	3.37802900	2.70319100	-1.67830100
C	0.81518200	1.39995600	-4.14031500
C	1.05052500	3.59230200	-3.04338700
C	2.86230500	4.03766600	-1.47283300
C	-0.29773500	1.84987100	-4.80125200
H	1.13622800	0.37345500	-4.26391800
C	-0.11473000	4.02281800	-3.75253000
C	1.71368100	4.44485900	-2.15702700
C	-0.76752600	3.18132100	-4.61400200
H	-0.84162800	1.17399300	-5.45381500

H	-0.46330700	5.04152700	-3.59643900
H	1.32226700	5.44551200	-1.98808300
H	-1.64492700	3.52450600	-5.15716500
C	0.60351600	-3.58004000	2.38812000
C	0.04426800	-2.70273600	3.34781500
C	-0.17603900	-4.62754700	1.84063100
C	0.77584600	-1.61418200	3.92511400
C	-1.32501000	-2.88787700	3.77215200
C	-1.54734500	-4.79461200	2.26546600
C	0.21034300	-0.79066300	4.86409900
H	1.79329600	-1.43558100	3.59774300
C	-1.87691200	-2.00720000	4.75555300
C	-2.08200100	-3.92440500	3.21985500
C	-1.13388800	-0.99088700	5.29186900
H	0.78931200	0.03067300	5.27629300
H	-2.90612800	-2.16789700	5.06899400
H	-3.11076900	-4.06287400	3.54735000
H	-1.56462800	-0.33054000	6.03994600
C	5.20207600	3.22466200	-0.13336200
H	6.10964100	2.92327500	0.38264400
C	4.57914000	2.34824100	-0.98263700
H	5.00412900	1.36379400	-1.13982700
C	4.67579600	4.52959000	0.08032200
H	5.18188600	5.21001300	0.75990900
C	3.54190600	4.92270200	-0.57744500
H	3.12782500	5.91539900	-0.42277900
C	-0.43375300	-6.57508700	0.38633100
H	-0.01362700	-7.27002100	-0.33577400
C	-1.78764500	-6.72759200	0.79907400
H	-2.38834600	-7.53485500	0.38876100
C	-2.32320400	-5.86278800	1.71487300
H	-3.35221700	-5.97626100	2.04865500
C	0.34282300	-5.56546400	0.89152400
H	1.37399900	-5.46883100	0.57131300
N	0.42069100	-1.00771400	-1.82079800
S	-1.04329900	-1.48619000	-2.12434100
O	-1.64632000	-0.72635400	-3.23197700
O	-1.90682600	-1.66539100	-0.91730800
C	-0.89024100	-3.22206300	-2.80331500
F	-0.12246400	-3.21604600	-3.89777700
F	-2.10993000	-3.67035100	-3.13261400
F	-0.35640400	-4.04304800	-1.89839000
C	-5.29317700	-0.18743900	-0.71434100
C	-4.52815500	0.33391500	-1.96984200

H	-5.19988300	0.31777200	-2.83989900
H	-3.72757800	-0.36422300	-2.21466100
C	-3.93554400	1.69619300	-1.90722500
C	-4.44170900	0.13138600	0.56874500
H	-4.91702500	0.90841100	1.16163000
H	-4.37333700	-0.77112300	1.18516800
N	-3.06992000	0.59585800	0.31452300
C	-2.49969900	1.65645100	0.94603900
N	-1.16276400	1.63463700	1.06837000
C	-0.30539800	2.66445500	1.54433900
C	-0.41871500	3.99639500	1.14145400
C	0.74029500	2.27590000	2.39114100
C	0.48366000	4.94207500	1.63016200
C	1.64019700	3.23032500	2.85812900
H	0.84370300	1.23303600	2.66561000
C	1.51149200	4.57148700	2.49445500
H	2.21215300	5.31050800	2.86411600
C	2.80503600	2.81923400	3.72055700
C	0.31669100	6.38548500	1.23616300
F	2.60841800	1.61621400	4.30696500
F	3.94774600	2.73101100	3.00689000
F	3.02852700	3.71818900	4.70684600
F	1.48859400	7.06083100	1.28014800
F	-0.17088700	6.50985900	-0.02213300
F	-0.54174500	7.03550200	2.05202300
S	-3.48774000	2.98368500	1.45675500
H	-1.19068500	4.29643600	0.44719200
H	-0.65911900	0.73317600	0.91427800
H	-2.44054000	-0.14287200	-0.04004500
C	-4.54502100	2.85617500	-1.41998600
H	-5.62653300	2.84121400	-1.28139400
H	-4.16074400	2.91966800	-0.19869200
H	-4.13843700	3.80277700	-1.77975600
C	-5.38659800	-1.74825800	-0.91481900
H	-4.36718600	-2.13505000	-1.01949700
H	-5.90065300	-1.91942400	-1.87148700
C	-6.72570200	0.37561600	-0.57993000
C	-7.34168200	0.50811500	0.67739700
C	-7.50954100	0.67809500	-1.70646200
C	-8.65909700	0.95136400	0.80430600
H	-6.80221200	0.24833500	1.58206300
C	-8.82644300	1.12463800	-1.58498300
H	-7.10359300	0.56681500	-2.70709000
C	-9.40885900	1.27007000	-0.32669700

H	-9.09651700	1.04411700	1.79471400
H	-9.39529400	1.35700300	-2.48136100
H	-10.43270600	1.61997900	-0.22990000
C	-6.10076400	-2.50581200	0.17027300
C	-5.51134800	-3.40343900	0.96426400
H	-4.45372300	-3.64278200	0.87365700
H	-6.07160500	-3.94372900	1.72366100
H	-2.93271100	1.78388400	-2.32737500
H	-7.16500700	-2.30686700	0.28991900

TS-EF-3RR-2

1 imaginary frequency

H = -5236.776494

G = -5236.970888

E(M06-2X-DCM) = -5237.614010

E(M06-2X-cyclohexane) = -5237.585092

O	1.15439700	-2.77878700	0.06217500
O	2.79054800	-0.79901200	-0.19491700
P	1.20111300	-1.15493700	-0.15983500
O	0.59210200	-0.39796500	0.97962400
C	2.98708800	-4.31499800	3.50034400
C	3.72287700	-4.09363700	2.34090100
C	3.09792700	-3.63465700	1.17134900
C	0.96678000	-3.53874500	2.36019200
C	1.61657800	-4.05736100	3.49281500
C	3.59059300	-1.31105700	-1.21894600
C	4.04861900	-2.62469500	-1.14523100
C	4.68214800	-3.18688000	-2.26501700
C	4.97211000	-2.40876400	-3.38087100
C	4.62909900	-1.05567800	-3.37325900
C	3.91971800	-0.47950500	-2.30724200
H	1.02782800	-4.23484900	4.38816800
H	4.88992700	-0.42650400	-4.21919100
C	4.09362300	-3.61584700	0.01583500
C	5.43461900	-3.46050900	0.81479400
H	5.58221300	-2.39992600	1.04883300
H	6.30335300	-3.79933300	0.24219300
H	6.01515700	-4.85546300	-1.86953500
H	4.64983100	-5.27389700	-2.89815700
C	1.74122900	-3.31824500	1.20543500
H	3.46953000	-4.67727900	4.40466200
H	5.47101300	-2.84002300	-4.24523100
C	5.21077400	-4.25162300	2.12040900
H	5.80409300	-3.86582800	2.95717100

H	5.48513000	-5.30927800	1.99992100
C	4.94690800	-4.66088900	-2.03945500
C	4.11057100	-4.96495700	-0.77537400
H	3.08331400	-5.21808800	-1.06164800
H	4.50737400	-5.79412500	-0.18081700
C	3.57871200	0.97679800	-2.32610200
C	2.70373200	1.49645800	-3.31142100
C	4.18641100	1.84576900	-1.38389000
C	2.04153100	0.67235300	-4.27784800
C	2.43491600	2.91700900	-3.34784100
C	3.87941300	3.25753700	-1.41181500
C	1.21700600	1.21168300	-5.22950200
H	2.17250800	-0.40148300	-4.22756400
C	1.57074100	3.43940100	-4.36102600
C	3.01449400	3.75411200	-2.39102900
C	0.98524100	2.61533000	-5.28334500
H	0.71508200	0.55876500	-5.93774300
H	1.39294200	4.51249500	-4.38020000
H	2.78314500	4.81670000	-2.40354900
H	0.33273500	3.02453200	-6.05049300
C	-0.50076800	-3.25453900	2.42973800
C	-0.97479000	-2.22568400	3.27967600
C	-1.41475700	-4.06065900	1.70875200
C	-0.09896600	-1.33926900	3.98749100
C	-2.39767900	-2.02830000	3.43853500
C	-2.83501100	-3.83870500	1.85814600
C	-0.58610600	-0.35461100	4.80759900
H	0.97005400	-1.44317100	3.84747900
C	-2.86534700	-0.99934200	4.31691500
C	-3.28643200	-2.84225500	2.72942000
C	-1.98999500	-0.18608700	4.98476700
H	0.10424800	0.31293000	5.31658900
H	-3.93946100	-0.87744300	4.44076500
H	-4.35769100	-2.70681700	2.86938800
H	-2.35960300	0.59325100	5.64590000
C	5.67896900	2.25855200	0.50985300
H	6.38206000	1.88485500	1.24934300
C	5.12193800	1.39569600	-0.39687900
H	5.39682900	0.34753300	-0.37459700
C	5.34778000	3.64276500	0.49570800
H	5.79494900	4.31041000	1.22736200
C	4.47745400	4.12517000	-0.44370100
H	4.21525500	5.17905000	-0.47074400
C	-1.90572200	-5.88131800	0.15479200

H	-1.55914700	-6.67481000	-0.50173400
C	-3.30288400	-5.64519400	0.29138700
H	-4.00906800	-6.25635500	-0.26424900
C	-3.75129700	-4.65583300	1.12414200
H	-4.81616600	-4.46640200	1.23605600
C	-0.99689200	-5.11995700	0.84132500
H	0.06290200	-5.31739800	0.72972100
N	0.66236900	-0.92881900	-1.67065200
S	-0.81063600	-1.17395700	-2.15528300
O	-1.23896800	-0.19495400	-3.16889200
O	-1.79650100	-1.43700500	-1.06186100
C	-0.73938800	-2.79084600	-3.08997000
F	0.12927700	-2.69056200	-4.10304100
F	-1.95202700	-3.06917100	-3.58788900
F	-0.36056200	-3.78737800	-2.28806000
C	-5.20342200	0.18993700	-0.80720100
C	-4.36865900	0.49367900	-2.08742400
H	-5.01876100	0.43257300	-2.97114700
H	-3.62988600	-0.29818000	-2.21384300
C	-3.65017700	1.79733500	-2.15673200
C	-4.31161000	0.50380500	0.45503600
H	-4.72721600	1.33033300	1.02543600
H	-4.27107300	-0.37412700	1.10764700
N	-2.91593100	0.86650400	0.16788800
C	-2.28242500	1.93664000	0.71521700
N	-0.95575300	1.83429800	0.88135900
C	-0.05385800	2.85060100	1.30530800
C	-0.00295500	4.11148400	0.70597700
C	0.84641300	2.51933100	2.32177000
C	0.92088300	5.05052900	1.16205000
C	1.76995400	3.46695200	2.76150100
H	0.81441400	1.52843900	2.75935800
C	1.80726000	4.73946800	2.19430300
H	2.51072300	5.48024700	2.55509900
C	2.75807700	3.09596100	3.83727100
C	1.00246300	6.40162800	0.50201400
F	2.24013200	2.19313500	4.70250400
F	3.88045500	2.55061900	3.32355000
F	3.13663900	4.17547200	4.55799800
F	1.30150300	7.37290800	1.39054200
F	1.96913000	6.44171600	-0.45277000
F	-0.15415800	6.74120600	-0.10432000
S	-3.18158700	3.37648500	1.05883000
H	-0.67882600	4.36280900	-0.09973800

H	-0.50997500	0.88974800	0.84759700
H	-2.32988100	0.07321900	-0.13823700
C	-4.15574500	3.05344500	-1.82271600
H	-5.23509400	3.16367500	-1.71831400
H	-3.80466800	3.20345100	-0.57779500
H	-3.64026900	3.91541500	-2.24881400
C	-5.50139300	-1.35455800	-0.87079700
H	-4.53157000	-1.87210400	-0.85529600
H	-5.96555700	-1.57308400	-1.84016400
C	-6.55021100	0.94396100	-0.75164600
C	-7.16568900	1.25007900	0.47392900
C	-7.26745200	1.25718000	-1.91830500
C	-8.41467800	1.86934900	0.53230900
H	-6.68136600	0.99613600	1.41106200
C	-8.51718300	1.87695300	-1.86653700
H	-6.86025000	1.02101400	-2.89635500
C	-9.09704200	2.19333400	-0.63896700
H	-8.85305100	2.09418900	1.50086500
H	-9.03488900	2.11111400	-2.79297900
H	-10.06784100	2.67896900	-0.59616900
C	-6.37767100	-1.90309800	0.22177000
C	-7.51375400	-2.57281400	0.02196500
H	-7.90536800	-2.74982700	-0.97756100
H	-8.09569400	-2.97170000	0.84846700
H	-2.63239900	1.73074700	-2.54232100
H	-6.03201700	-1.76010700	1.24613000

TS-EF-3RR-3

1 imaginary frequency

H = -5236.767515

G = -5236.962726

E(M06-2X-DCM) = -5237.608786

E(M06-2X-cyclohexane) = -5237.579822

O	-2.48034200	-1.18183700	-0.99578200
O	-1.94257400	-1.28227700	1.54215100
P	-1.39582200	-0.68429000	0.11763600
O	-1.33215300	0.80457300	0.29357000
C	-6.59763400	-0.50418000	-0.63299200
C	-5.98650400	-1.54494700	0.05707200
C	-4.61824700	-1.81324100	-0.10899900
C	-4.44039200	0.10082200	-1.61966000
C	-5.82784800	0.28550100	-1.48420400
C	-1.91961300	-2.66133200	1.75984000
C	-2.90557800	-3.46623900	1.19295000

C	-2.75476000	-4.86190200	1.23595100
C	-1.71675900	-5.44145600	1.95635600
C	-0.82631400	-4.61569000	2.64259800
C	-0.89306600	-3.21598300	2.54891300
H	-6.29839900	1.08194300	-2.05277300
H	-0.03752800	-5.05424800	3.24658000
C	-4.26436600	-3.12631100	0.58580500
C	-5.36931800	-3.15133300	1.69848200
H	-5.03639000	-2.52779700	2.53643900
H	-5.55017900	-4.15865500	2.08486200
H	-4.57270500	-6.03737900	1.05165400
H	-3.42051800	-6.30772400	-0.25132300
C	-3.84844800	-0.95182200	-0.89093500
H	-7.66119300	-0.30990000	-0.51947600
H	-1.60245400	-6.52169100	1.99768700
C	-6.60759200	-2.51412500	1.03736600
H	-7.26663400	-2.01744800	1.75871100
H	-7.21808300	-3.26712400	0.51940000
C	-3.83040200	-5.53849100	0.41309400
C	-4.45248300	-4.35611800	-0.36338600
H	-3.88142700	-4.17961300	-1.28094100
H	-5.49912000	-4.51785400	-0.63973500
C	0.07775400	-2.38717500	3.33048400
C	1.46332100	-2.45346200	3.04300900
C	-0.38265000	-1.62893100	4.43752300
C	1.98732700	-3.17267600	1.92013000
C	2.40552300	-1.76442500	3.89754500
C	0.56903600	-0.92125400	5.26453900
C	3.33545900	-3.24014100	1.68489700
H	1.29886700	-3.64302500	1.23035100
C	3.80567300	-1.87190100	3.62321500
C	1.93355700	-1.01271500	4.97619700
C	4.26242700	-2.59776700	2.55546100
H	3.69939300	-3.77187800	0.81107000
H	4.50064000	-1.36434600	4.28869600
H	2.64669600	-0.49541200	5.61536800
H	5.32661800	-2.66836000	2.35157400
C	-3.68254100	1.00179400	-2.54251800
C	-3.68656800	2.40249300	-2.31227200
C	-3.05728200	0.47606100	-3.70168200
C	-4.29684500	3.00590800	-1.16341400
C	-3.05967600	3.28734100	-3.27015200
C	-2.39267900	1.36982500	-4.62380000
C	-4.35020200	4.36800800	-1.00847300

H	-4.72629200	2.36472000	-0.40300600
C	-3.13082400	4.70249400	-3.06883800
C	-2.41438300	2.74652900	-4.38590300
C	-3.77205300	5.23439100	-1.98089000
H	-4.83711200	4.79233700	-0.13429200
H	-2.67643200	5.34985300	-3.81587300
H	-1.94019400	3.41569900	-5.10161900
H	-3.84267900	6.31201200	-1.85555300
C	-2.17422400	-0.82198000	5.89612100
H	-3.22901200	-0.78830800	6.15585700
C	-1.76352000	-1.55265900	4.81122500
H	-2.49509100	-2.09689600	4.22543600
C	-1.23294000	-0.11180500	6.69459500
H	-1.57588500	0.45958100	7.55309900
C	0.09895200	-0.16432400	6.38350900
H	0.83183900	0.36216100	6.99072500
C	-2.46422700	-1.39050900	-5.16129300
H	-2.48833800	-2.45438400	-5.37944400
C	-1.78261500	-0.50958900	-6.04674700
H	-1.29142100	-0.90784200	-6.93015400
C	-1.75453400	0.83238400	-5.78498900
H	-1.25044500	1.52029800	-6.45975600
C	-3.08080800	-0.91537900	-4.03499500
H	-3.59578400	-1.60527800	-3.37846100
N	-0.01679100	-1.44747800	-0.23892600
S	0.53157600	-1.95248700	-1.65193000
O	1.94793000	-2.30866200	-1.47368400
O	0.16534900	-1.11133300	-2.80132900
C	-0.28050200	-3.61475000	-1.97578700
F	-0.22101700	-4.38753800	-0.88177100
F	0.37189200	-4.22582900	-2.96951700
F	-1.56686200	-3.48289800	-2.33248000
C	-0.40572900	4.12503900	1.23699600
C	-0.69719500	3.86791400	-0.27354400
H	-1.36069800	4.64977300	-0.66866100
H	-1.26236600	2.93884800	-0.36149200
C	0.46773400	3.78974300	-1.18830700
C	0.75626000	3.16702900	1.68462900
H	1.67312600	3.72189000	1.86588700
H	0.47068800	2.66963300	2.61767600
N	1.09869900	2.12266300	0.70790100
C	2.36820500	1.78876900	0.37077600
N	2.58728700	0.54323800	-0.09124100
C	3.82348800	0.11612600	-0.68460000

C	3.88933500	-0.08063900	-2.06332000
C	4.93412800	-0.12359800	0.12105400
C	5.08891100	-0.50249100	-2.63689800
C	6.12847600	-0.54698700	-0.46403400
H	4.86160400	0.01003700	1.19342300
C	6.21217700	-0.73457100	-1.84314700
H	7.14092600	-1.06327500	-2.29472800
C	7.31263600	-0.86529100	0.40915300
C	5.19552200	-0.64551200	-4.13324400
F	7.29093700	-2.15651600	0.82970600
F	8.48115600	-0.68997400	-0.24280500
F	7.34084900	-0.09650800	1.51838300
F	5.63596100	0.50284700	-4.70398100
F	6.07196100	-1.61362900	-4.48006200
F	4.01028000	-0.93822400	-4.69946900
S	3.62450000	2.97508800	0.40497000
H	3.00833200	0.07052300	-2.67572700
H	1.83606400	-0.15534600	-0.03240200
H	0.33943300	1.43539500	0.54261400
C	1.59111400	4.62879000	-1.20873200
H	1.52147500	5.57285900	-0.66777400
H	2.44432400	4.01040600	-0.51614500
H	2.13246600	4.68157200	-2.15509700
C	-1.73225300	3.72981600	1.98984500
H	-1.95717000	2.68704200	1.74201100
H	-2.53823500	4.34473300	1.56619400
C	-0.07850700	5.59821100	1.56239300
C	0.77500700	5.94580600	2.62391500
C	-0.70550500	6.65319400	0.87661700
C	1.01740100	7.27878200	2.96097900
H	1.25338300	5.17482900	3.21860000
C	-0.46383900	7.98707600	1.20807500
H	-1.40154900	6.44693000	0.06924400
C	0.40525400	8.30940600	2.24998400
H	1.68754600	7.50596700	3.78572800
H	-0.96052500	8.77463300	0.64735900
H	0.59670000	9.34730700	2.50747200
C	-1.70424800	3.90036600	3.48363900
C	-1.79348400	2.88984400	4.35224300
H	-1.78180100	3.05828700	5.42595600
H	-1.89198200	1.85610000	4.02762400
H	-1.61486400	4.91894800	3.85994800
H	0.41288800	3.00935600	-1.94807600

TS-EF-3RR-4

1 imaginary frequency

H = -5236.763423

G = -5236.957913

E(M06-2X-DCM) = -5237.605529

E(M06-2X-cyclohexane) = -5237.577547

O	-2.98581000	-0.81246300	-0.84676000
O	-2.27416900	-1.45386000	1.56363300
P	-1.90845500	-0.44300400	0.32881100
O	-1.99414300	0.94344600	0.85714500
C	-7.06602700	-0.36961000	-0.03184600
C	-6.39078000	-1.52971600	0.33293000
C	-5.03879200	-1.70566500	0.00117800
C	-5.01083200	0.51065900	-1.02740800
C	-6.38000100	0.62310200	-0.73099300
C	-2.17315700	-2.83495800	1.40921400
C	-3.18065600	-3.53176100	0.74345000
C	-2.98035500	-4.88624400	0.43073900
C	-1.86160700	-5.56532500	0.89976800
C	-0.93642900	-4.88197600	1.68866600
C	-1.05559400	-3.50602800	1.94651300
H	-6.90274900	1.52130000	-1.04647300
H	-0.08286600	-5.41173500	2.10086200
C	-4.59746100	-3.12596100	0.33920900
C	-5.60989100	-3.45885100	1.48969000
H	-5.22277700	-3.04335100	2.42731300
H	-5.74136600	-4.53559200	1.63249200
H	-4.77386200	-6.07122200	0.11827800
H	-3.73481700	-5.97612700	-1.29935300
C	-4.35123100	-0.66353900	-0.61628600
H	-8.11597800	-0.23590900	0.21629400
H	-1.71124400	-6.61698600	0.66915200
C	-6.91045500	-2.72731500	1.09671200
H	-7.51591200	-2.44321400	1.96501800
H	-7.54791300	-3.35769300	0.46069900
C	-4.10461800	-5.40298500	-0.44143100
C	-4.82477500	-4.10273500	-0.86192100
H	-4.33606300	-3.68273200	-1.74837900
H	-5.88503700	-4.24506000	-1.09366100
C	-0.04148400	-2.83534700	2.81890000
C	1.32540400	-2.82118500	2.44138500
C	-0.43314100	-2.31625200	4.08106700
C	1.78942700	-3.29970200	1.17187500
C	2.31619400	-2.30313800	3.35922300

C	0.56408600	-1.75611300	4.96524900
C	3.12559200	-3.32750000	0.86432500
H	1.06348600	-3.62578300	0.43750500
C	3.70010100	-2.35317400	2.99922100
C	1.90849900	-1.77238400	4.58502000
C	4.10127300	-2.86683200	1.79552100
H	3.44388300	-3.69391900	-0.10766500
H	4.42977400	-1.98171500	3.71554300
H	2.65777400	-1.37640600	5.26797700
H	5.15691900	-2.90461100	1.54058100
C	-4.33393700	1.60757000	-1.78754900
C	-4.22077700	2.89810800	-1.21373600
C	-3.89226200	1.37846900	-3.11457300
C	-4.62715100	3.19076200	0.12892600
C	-3.67092000	3.98280600	-1.99625300
C	-3.31272500	2.46441900	-3.87214100
C	-4.54766200	4.46021900	0.64036400
H	-4.99291500	2.38214600	0.75028400
C	-3.60257400	5.29317100	-1.42434400
C	-3.22378500	3.73465100	-3.29661600
C	-4.03828000	5.53260800	-0.14761900
H	-4.86961800	4.65227600	1.66042400
H	-3.20871800	6.10109100	-2.03744400
H	-2.80796300	4.55351400	-3.88096100
H	-3.99798000	6.53606100	0.26850800
C	-2.12877800	-1.83614400	5.77780100
H	-3.16387800	-1.87575000	6.10643500
C	-1.78448800	-2.34846900	4.55443500
H	-2.54854800	-2.79623300	3.93059900
C	-1.14612700	-1.25524900	6.62800600
H	-1.43863100	-0.84959600	7.59274800
C	0.16250900	-1.22358800	6.23045800
H	0.92883500	-0.79846400	6.87455100
C	-3.58277600	-0.07632400	-5.05304000
H	-3.68711800	-1.05163400	-5.52047000
C	-2.99002400	0.99080800	-5.78486400
H	-2.64438100	0.82051300	-6.80083000
C	-2.86479900	2.22510900	-5.20868900
H	-2.42456600	3.05327200	-5.75930400
C	-4.02053300	0.11205900	-3.76897300
H	-4.47548600	-0.71192900	-3.23254500
N	-0.47611700	-0.93847100	-0.28377200
S	-0.04821500	-1.02850900	-1.80672000
O	1.40115200	-1.36484100	-1.82902300

O	-0.48630800	0.07677100	-2.67381100
C	-0.79248500	-2.59232600	-2.55028300
F	-0.71216500	-3.59852600	-1.66909400
F	-0.09312100	-2.91485000	-3.64192500
F	-2.07152800	-2.42672800	-2.89761200
C	0.19901700	3.70371400	1.33264700
C	-0.27070200	3.50018900	-0.14971300
H	-0.86164600	4.37431800	-0.45453100
H	-0.95527400	2.64953200	-0.17224700
C	0.79557100	3.29744600	-1.17707200
C	1.01425200	2.42249300	1.75485200
H	1.87955600	2.67099500	2.36329400
H	0.35617400	1.79589700	2.35838200
N	1.48788700	1.52373200	0.67198400
C	2.77607800	1.32607000	0.31454300
N	3.08982400	0.17240900	-0.29542600
C	4.36354600	-0.19264600	-0.81500100
C	4.45033400	-0.61949200	-2.14307700
C	5.49132700	-0.21418600	0.00637400
C	5.67996100	-1.04535400	-2.64710700
C	6.71148700	-0.64734700	-0.51061400
H	5.41134600	0.07783900	1.04614200
C	6.81666600	-1.05921400	-1.83876100
H	7.76941100	-1.38672900	-2.23683100
C	7.88963500	-0.76571300	0.41907600
C	5.76656400	-1.54874200	-4.06597100
F	7.81430300	-1.90505000	1.15289700
F	9.06190500	-0.79924700	-0.24559700
F	7.94155000	0.25860200	1.29663100
F	7.00022000	-1.36137300	-4.58476000
F	5.50438900	-2.87251000	-4.13692100
F	4.88386000	-0.92434200	-4.87244800
S	3.91455300	2.62439500	0.47197200
H	3.56192000	-0.62660100	-2.76407700
H	2.33011700	-0.46916300	-0.58085400
H	0.83840000	0.75681400	0.45761800
C	1.93559800	4.06657700	-1.35192700
H	1.97629100	5.05965500	-0.90776300
H	2.81586900	3.48228600	-0.48668100
H	2.48801400	3.94201600	-2.28314300
C	-1.11557400	3.72864100	2.17920100
H	-1.68202100	2.82481200	1.92539600
H	-1.73764200	4.56179400	1.82576400
C	0.92576100	5.06286100	1.50556700

C	2.17965700	5.23190700	2.10874400
C	0.26890200	6.22999100	1.06971900
C	2.75850700	6.49603600	2.25491400
H	2.74297900	4.37934900	2.46565800
C	0.84092100	7.49276600	1.21154000
H	-0.71384100	6.16174100	0.61170700
C	2.09637500	7.63497400	1.80468100
H	3.73492000	6.58044200	2.72474300
H	0.30030100	8.36726400	0.85873900
H	2.54666700	8.61739100	1.91640000
C	-1.05028900	3.81379900	3.68335000
C	-0.00738200	3.90722900	4.50973400
H	-0.15612700	3.93943400	5.58575000
H	1.02082700	3.96870000	4.17108400
H	-2.04313300	3.77038000	4.13532400
H	0.63883900	2.45757100	-1.85560200

TS-EF-3RR-5

1 imaginary frequency

H = -5236.767926

G = -5236.963488

E(M06-2X-DCM) = -5237.611213

E(M06-2X-cyclohexane) = -5237.580904

O	2.26730200	-1.87065300	-0.01037200
O	1.94076700	0.15566900	-1.59602900
P	1.27061900	-0.62153700	-0.31305700
O	1.20913200	0.41309300	0.77302900
C	6.34165400	-1.27625400	0.72494400
C	5.85720000	-1.32389900	-0.57803400
C	4.50069000	-1.58240000	-0.83135800
C	4.08183600	-1.66333100	1.57724400
C	5.45800200	-1.47331600	1.78607800
C	2.00083700	-0.47874800	-2.83615700
C	2.98681500	-1.43419900	-3.07638300
C	2.91090000	-2.21027100	-4.24461600
C	1.95618100	-1.93750800	-5.21782500
C	1.06984900	-0.87834000	-5.02022300
C	1.05706300	-0.13946700	-3.82628100
H	5.82830700	-1.46350300	2.80706800
H	0.34638100	-0.62749600	-5.79036700
C	4.27683000	-1.77267100	-2.32952200
C	5.46762900	-0.91978500	-2.89068500
H	5.16715700	0.13442800	-2.90498800
H	5.73884500	-1.20218400	-3.91225200

H	4. 77217800	-3. 09522700	-4. 93215600
H	3. 54252900	-4. 27931600	-4. 50254500
C	3. 62353400	-1. 68982800	0. 24534200
H	7. 39531500	-1. 09196500	0. 91920900
H	1. 90196400	-2. 53203200	-6. 12625800
C	6. 61020600	-1. 11897200	-1. 87355700
H	7. 29511600	-0. 26431000	-1. 83204600
H	7. 21927300	-1. 99925800	-2. 12297200
C	3. 95765200	-3. 30388700	-4. 22456800
C	4. 45336300	-3. 26615500	-2. 76144200
H	3. 80234200	-3. 88842100	-2. 13807600
H	5. 48182500	-3. 62033200	-2. 63963900
C	0. 09330400	0. 99715800	-3. 67727700
C	-1. 30289300	0. 75308300	-3. 66304600
C	0. 58026200	2. 32973600	-3. 65134000
C	-1. 85795200	-0. 56710700	-3. 64316900
C	-2. 22562600	1. 86766000	-3. 64555000
C	-0. 35454900	3. 43280200	-3. 60540900
C	-3. 21284200	-0. 77024700	-3. 63681100
H	-1. 18944300	-1. 41605200	-3. 59332700
C	-3. 63336200	1. 61127600	-3. 65676100
C	-1. 72820600	3. 17265400	-3. 61153600
C	-4. 11709400	0. 32993400	-3. 65905900
H	-3. 60093800	-1. 78273600	-3. 58690900
H	-4. 31112700	2. 46213000	-3. 66091500
H	-2. 42703900	4. 00697100	-3. 59652200
H	-5. 18725300	0. 14480000	-3. 64764000
C	3. 16347700	-1. 84343000	2. 74375900
C	2. 98889200	-0. 78893500	3. 67468300
C	2. 51026000	-3. 08471200	2. 94434200
C	3. 63568200	0. 48367900	3. 54654700
C	2. 12492700	-0. 98260000	4. 81815600
C	1. 63354800	-3. 25541700	4. 08028800
C	3. 47782000	1. 46774000	4. 48949400
H	4. 26695600	0. 66382000	2. 68423700
C	1. 97167700	0. 07654700	5. 76795000
C	1. 46290700	-2. 20213100	4. 98184100
C	2. 63441300	1. 26588000	5. 61971600
H	4. 00327900	2. 41303000	4. 37561400
H	1. 32437900	-0. 09410100	6. 62547600
H	0. 80872700	-2. 34021400	5. 84059800
H	2. 52553200	2. 05313500	6. 36142000
C	2. 41509700	3. 95016000	-3. 67397200
H	3. 48053600	4. 15996100	-3. 71316800

C	1. 97538100	2. 65193000	-3. 69908800
H	2. 69578300	1. 84501300	-3. 76509000
C	1. 48999100	5. 03089300	-3. 60590200
H	1. 85540300	6. 05438800	-3. 59513700
C	0. 14476900	4. 77415000	-3. 57715200
H	-0. 57566500	5. 58904000	-3. 55102900
C	2. 05219200	-5. 39622000	2. 30318600
H	2. 20963700	-6. 23119400	1. 62603500
C	1. 16913400	-5. 54929900	3. 40870800
H	0. 65729500	-6. 49525500	3. 56198500
C	0. 97130500	-4. 50770100	4. 27248300
H	0. 30578700	-4. 61194300	5. 12605000
C	2. 69890800	-4. 21005600	2. 08054700
H	3. 37022800	-4. 11697500	1. 23511100
N	-0. 12793400	-1. 26859700	-0. 80010100
S	-0. 76213200	-2. 69880900	-0. 43795900
O	-2. 15406900	-2. 69634800	-0. 90784100
O	-0. 47756900	-3. 17090600	0. 92363000
C	0. 07182300	-3. 94549000	-1. 57201000
F	0. 13831100	-3. 47537600	-2. 82758700
F	-0. 65003800	-5. 07023600	-1. 57439200
F	1. 31410200	-4. 23918100	-1. 16503900
C	0. 67734100	4. 03238800	1. 29514200
C	0. 85429800	3. 08123000	2. 51618000
H	1. 49224800	3. 56094200	3. 27151300
H	1. 40388500	2. 19841100	2. 18563000
C	-0. 37410200	2. 60554200	3. 20708000
C	-0. 54519200	3. 52994200	0. 44317100
H	-1. 41446500	4. 16447300	0. 60606100
H	-0. 29097500	3. 57719300	-0. 62205600
N	-0. 95038400	2. 15239800	0. 74596300
C	-2. 23945400	1. 72466000	0. 77023100
N	-2. 45847300	0. 43869000	0. 44293000
C	-3. 70344000	-0. 25427100	0. 59507600
C	-3. 76392100	-1. 35930500	1. 44412600
C	-4. 82112600	0. 13664200	-0. 13924500
C	-4. 96310900	-2. 06062800	1. 57018700
C	-6. 01442700	-0. 57371600	-0. 00514600
H	-4. 75339500	0. 97311300	-0. 82356500
C	-6. 09294700	-1. 67123000	0. 85085000
H	-7. 02043600	-2. 22253000	0. 95002100
C	-7. 19649100	-0. 18588600	-0. 85286600
C	-5. 06101800	-3. 20956000	2. 54054400
F	-7. 11415000	-0. 71897700	-2. 09857400

F	-8.36192400	-0.61064200	-0.32214400
F	-7.28064900	1.15295800	-1.01088700
F	-5.48677200	-2.78557900	3.75675100
F	-5.94555500	-4.14111200	2.12213300
F	-3.87581500	-3.81737100	2.72714900
S	-3.48732800	2.77005700	1.34259200
H	-2.87857600	-1.68517700	1.97871300
H	-1.69310900	-0.09362600	0.00028000
H	-0.21104300	1.43483600	0.61183300
C	-1.48690000	3.36119600	3.60497000
H	-1.38745600	4.44702700	3.60258600
H	-2.32899300	3.18098800	2.68096600
H	-2.06270800	2.95667600	4.43971000
C	1.97612500	3.90271300	0.41748700
H	1.86887400	4.56332500	-0.44961100
H	2.01460600	2.87334100	0.03740000
C	0.46568900	5.51585700	1.64467200
C	0.07564400	6.40214300	0.62392400
C	0.68573900	6.05841000	2.91774100
C	-0.10367800	7.76213600	0.86912300
H	-0.08319400	6.02883800	-0.38456100
C	0.50634000	7.42179100	3.16911500
H	1.00292700	5.42543400	3.74020600
C	0.10838300	8.28090200	2.14766100
H	-0.40913300	8.41735800	0.05762800
H	0.68287200	7.80716200	4.16987100
H	-0.03191700	9.34043800	2.34237700
C	3.26171100	4.21576400	1.13348000
C	4.02012700	5.28896700	0.90482100
H	4.94918300	5.45897500	1.44275400
H	3.74258200	6.03805500	0.16626700
H	3.58850700	3.48923100	1.87814000
H	-0.37057300	1.54819600	3.47082900

TS-1-1-3RS

1 imaginary frequency

H = -5236.769404

G = -5236.963926

E(M06-2X-DCM) = -5237.610978

C	4.41952900	-1.69647100	-0.95734300
C	3.65519200	-1.58940000	-2.32132300
H	3.85678200	-2.51622800	-2.87461500
H	4.07711000	-0.74671900	-2.87631400
C	2.17286600	-1.42740900	-2.28028700

C	4. 16165300	-0. 37903100	-0. 14799100
H	4. 24497600	-0. 58685700	0. 92323600
H	4. 92148600	0. 35574800	-0. 41337000
N	2. 86688500	0. 25519400	-0. 38695100
C	2. 75952900	1. 56455600	-0. 86675700
N	1. 47234200	2. 00928800	-0. 78611700
C	0. 89566900	3. 28601500	-0. 90094700
C	1. 56391500	4. 46963400	-1. 24754400
C	-0. 47575100	3. 34638100	-0. 59602100
C	0. 85951500	5. 67547400	-1. 27239000
C	-1. 15471400	4. 55925300	-0. 62002500
H	-1. 00001000	2. 43739400	-0. 32515000
C	-0. 49698300	5. 74206700	-0. 95798600
H	-1. 02477500	6. 68725600	-0. 97263300
C	-2. 59882500	4. 57105100	-0. 20133500
C	1. 57774900	6. 92598700	-1. 71125200
F	-3. 30249300	3. 57357700	-0. 78832000
F	-2. 73268000	4. 38884100	1. 14111800
F	-3. 21445000	5. 73212200	-0. 50199300
F	1. 01771600	8. 03755300	-1. 18112700
F	2. 87805400	6. 91598900	-1. 35070400
F	1. 54210800	7. 07281400	-3. 05625600
S	4. 06358400	2. 39970400	-1. 51481700
H	2. 61677900	4. 44680100	-1. 48720300
C	1. 24041800	-2. 42112700	-1. 97721700
H	0. 76216500	1. 27818400	-0. 64671900
H	1. 60800700	-3. 44399300	-1. 89180600
H	0. 27800000	-2. 30451700	-2. 48235200
H	2. 13745200	-0. 01375500	0. 26639700
H	0. 76325300	-2. 19409400	-0. 80552000
O	-2. 53341500	-1. 38572500	0. 05618900
O	-1. 11664300	0. 24338400	1. 50108200
P	-1. 04843700	-0. 76013400	0. 22315600
O	-0. 54500100	0. 07224100	-0. 90814700
C	-5. 60787900	1. 29074500	-0. 91669100
C	-5. 22427500	1. 10717200	0. 40677300
C	-4. 24892700	0. 15554000	0. 74929600
C	-3. 95814700	-0. 36662100	-1. 62338800
C	-4. 99216400	0. 53622500	-1. 91516500
C	-1. 53416000	-0. 11891300	2. 78801300
C	-2. 88457800	-0. 33854100	3. 04333700
C	-3. 24974600	-0. 88526200	4. 28394500
C	-2. 30421400	-1. 06709200	5. 28751100
C	-0. 98443000	-0. 67917700	5. 05720600

C	-0.56392200	-0.20653800	3.80394000
H	-5.28538600	0.66597900	-2.95279500
H	-0.25050900	-0.75480600	5.85390800
C	-4.14630100	0.03870200	2.26724500
C	-4.61672900	1.47915200	2.67493600
H	-4.96956200	1.52620900	3.70939200
H	-3.77016600	2.16818200	2.57453200
H	-5.27263000	-0.49257900	4.96461400
H	-4.93785100	-2.19975100	4.69499500
C	-3.59676300	-0.52560200	-0.27249700
H	-6.36725200	2.02341700	-1.17687300
H	-2.59015700	-1.48133000	6.25086600
C	-5.69377000	1.85243300	1.63549800
H	-5.75372700	2.93294300	1.46503400
H	-6.69322200	1.52108800	1.94982100
C	-4.73143700	-1.19331700	4.31378700
C	-5.14375900	-1.02456000	2.83451400
H	-4.99344100	-1.96797000	2.29744600
H	-6.18904900	-0.72699300	2.70576100
C	0.84540500	0.26134500	3.61419200
C	1.93077400	-0.63921800	3.76036500
C	1.09253500	1.63966800	3.37554600
C	1.75059500	-2.04521000	3.97170300
C	3.28796100	-0.14246900	3.68027500
C	2.45409600	2.11349300	3.26466900
C	2.82211400	-2.88840100	4.11422900
H	0.74546200	-2.44849700	3.99407500
C	4.37755300	-1.05509300	3.85215300
C	3.51155300	1.21402300	3.42876800
C	4.15499700	-2.38964600	4.06654800
H	2.65192200	-3.95190700	4.25268500
H	5.38987100	-0.65815100	3.81520100
H	4.53380100	1.58092900	3.36097600
H	4.99053600	-3.07189800	4.19896100
C	-3.28300300	-1.11052500	-2.73305800
C	-2.41982000	-0.42215600	-3.61962100
C	-3.55030600	-2.48839500	-2.91908200
C	-2.12493900	0.97481000	-3.49333000
C	-1.78783300	-1.14642200	-4.70055300
C	-2.90448600	-3.20146000	-3.99745100
C	-1.28565400	1.60683000	-4.37259900
H	-2.56814300	1.53559200	-2.67909400
C	-0.91495700	-0.44765900	-5.59367000
C	-2.03873300	-2.51352100	-4.85289600

C	-0.67130700	0.89024000	-5.43973000
H	-1.07672600	2.66602800	-4.25098600
H	-0.45350700	-1.00724600	-6.40423300
H	-1.55857600	-3.05318500	-5.66705400
H	-0.00995800	1.41127500	-6.12676700
C	0.32039800	3.93144800	3.00207900
H	-0.49952800	4.63539300	2.89294400
C	0.04786200	2.61214000	3.25391600
H	-0.98187900	2.29549900	3.36802900
C	1.66301600	4.38455600	2.86607400
H	1.86066400	5.43250600	2.65943200
C	2.69703900	3.49849800	3.00153800
H	3.72819700	3.83026300	2.90902500
C	-4.70461000	-4.55158500	-2.30201500
H	-5.40406800	-5.08070600	-1.66049600
C	-4.04864000	-5.25425300	-3.35241900
H	-4.24969900	-6.31178700	-3.50021200
C	-3.17584300	-4.59417800	-4.17461500
H	-2.67583800	-5.11641500	-4.98701800
C	-4.46344900	-3.21882300	-2.09329000
H	-4.97426600	-2.69819800	-1.29089600
N	-0.06550000	-2.06987700	0.42202000
S	-0.33729500	-3.46455700	1.23345500
C	-1.48409000	-4.47933200	0.12897200
O	0.91955700	-4.21642000	1.22029400
O	-1.08288400	-3.26888900	2.47824900
F	-1.25692700	-5.77285000	0.36859700
F	-1.22594600	-4.22472100	-1.16179800
F	-2.75841100	-4.20547700	0.39184000
C	5.94064300	-1.79485600	-1.19884500
C	6.80268200	-1.77047900	-0.08708400
C	6.52632100	-1.89922900	-2.46768700
C	8.18592100	-1.84145800	-0.23803800
H	6.39127900	-1.69262000	0.91555400
C	7.91325000	-1.97571600	-2.62261300
H	5.91100600	-1.92133300	-3.36043800
C	8.75061600	-1.94625400	-1.51023100
H	8.82286100	-1.81592700	0.64219900
H	8.33378200	-2.05644700	-3.62145600
H	9.82878900	-2.00374900	-1.63082000
C	3.96256000	-2.94545100	-0.14182800
H	4.52399700	-2.92989400	0.80244500
H	2.91131700	-2.86325100	0.15022400
C	4.21504900	-4.26520900	-0.82762900

C	3.37102900	-5.30032600	-0.84245700
H	2.40690300	-5.26368600	-0.34210000
H	3.63984700	-6.23490000	-1.32910900
H	5.18596500	-4.36819200	-1.31309600
H	1.77269200	-0.47937500	-2.63118200

TS-1-1-3SR

l imaginary frequency

H = -5236.776184

G = -5236.967472

E(M06-2X-DCM) = -5237.613406

C	2.88035900	3.59872000	0.44390600
C	2.12823900	3.79437900	1.81311800
H	2.84940000	3.62059600	2.61790100
H	1.79590300	4.83824200	1.85165700
C	0.92812600	2.94680800	2.04240300
C	1.84967000	3.78698800	-0.69981900
H	2.33921600	3.61230900	-1.66461900
H	1.47505600	4.81170000	-0.69370600
N	0.69816500	2.89729100	-0.59758300
C	-0.60205900	3.31316900	-0.85078900
N	-1.40458000	2.25113600	-1.15759400
C	-2.75224600	2.13148500	-1.52794100
C	-3.70920600	3.15668500	-1.51803400
C	-3.13753000	0.84366600	-1.94400900
C	-5.01456000	2.87922100	-1.92854500
C	-4.44130000	0.59242500	-2.35457500
H	-2.40787000	0.04022000	-1.94276600
C	-5.39712200	1.60916300	-2.35703000
H	-6.41048000	1.41758700	-2.68828200
C	-4.83398200	-0.81213900	-2.72239100
C	-6.05922600	3.96107200	-1.83210600
F	-5.90021300	-0.84643000	-3.54596500
F	-5.16639400	-1.54198600	-1.62127600
F	-3.82592000	-1.48155300	-3.32905800
F	-6.70491600	3.91559500	-0.63749500
F	-7.00643400	3.82969100	-2.78716600
F	-5.53187800	5.19511900	-1.94560800
S	-1.07694200	4.92144700	-0.70726800
C	3.52874100	2.17582800	0.37217700
H	4.05095000	2.10014200	-0.58732900
H	2.73759500	1.41834200	0.34726900
H	-3.43228300	4.15148100	-1.20089600
C	0.91283700	1.75619200	2.77931100

H	-0.92975000	1.34204500	-1.11153000
H	1.77253400	1.56186200	3.42421600
H	-0.04983300	1.49726500	3.22440800
H	0.88167400	1.91517800	-0.80924700
H	1.04967700	0.75014700	2.04102000
O	-1.22268500	-1.43990700	0.60286300
O	0.98666500	-2.43042200	-0.38582000
P	0.31997500	-1.07689800	0.21976900
O	0.23405900	0.04681200	-0.76557600
C	-2.13170500	-4.71020100	3.06586600
C	-1.76829900	-4.90456400	1.73820300
C	-1.55256000	-3.81013300	0.88706700
C	-2.00985800	-2.28612500	2.74260900
C	-2.29041800	-3.41004200	3.53950700
C	0.49511800	-2.85844800	-1.63546700
C	-0.67952400	-3.60450900	-1.66775700
C	-1.27676200	-3.87987000	-2.90876000
C	-0.65482900	-3.50394600	-4.09421400
C	0.57657800	-2.85119200	-4.03758500
C	1.17272700	-2.49769800	-2.81592700
H	-2.62443400	-3.24420700	4.55910100
H	1.08977300	-2.58162600	-4.95608500
C	-1.45171400	-4.30327500	-0.55472800
C	-0.89829700	-5.74819000	-0.31620300
H	-1.09691000	-6.41402600	-1.16184100
H	0.18767100	-5.69075700	-0.18060400
H	-3.39255000	-4.14138600	-3.34144800
H	-2.53623400	-5.64182900	-2.98446600
C	-1.58211500	-2.52242700	1.42051100
H	-2.31080600	-5.55672100	3.72369000
H	-1.11462400	-3.71949700	-5.05522000
C	-1.56375800	-6.20804900	0.99826000
H	-2.52116800	-6.71339200	0.80942300
H	-0.94143900	-6.91301800	1.56092400
C	-2.60484000	-4.57785500	-2.71864900
C	-2.87297300	-4.38293700	-1.21097200
H	-3.48736200	-5.17504400	-0.77253300
H	-3.39447600	-3.43261700	-1.05593300
C	2.50462100	-1.81248000	-2.82881200
C	3.66645400	-2.55406300	-2.50104300
C	2.61721100	-0.47187600	-3.26859200
C	3.62598300	-3.93816900	-2.13726800
C	4.96205900	-1.91680600	-2.56422400
C	3.92268400	0.14489200	-3.35178400

C	4. 76905100	-4. 62958800	-1. 83279000
H	2. 66755200	-4. 44391000	-2. 10614200
C	6. 12887500	-2. 66975000	-2. 22354500
C	5. 05429800	-0. 58668000	-2. 98263300
C	6. 03936100	-3. 98779600	-1. 86597000
H	4. 70825600	-5. 67963700	-1. 56009400
H	7. 09362900	-2. 16974200	-2. 26454600
H	6. 03368300	-0. 11591100	-3. 04067500
H	6. 93372700	-4. 55065600	-1. 61340900
C	-2. 24660500	-0. 92466400	3. 31945800
C	-3. 27949700	-0. 10640200	2. 79283800
C	-1. 52545500	-0. 50579000	4. 46788300
C	-4. 10535700	-0. 50109600	1. 69176500
C	-3. 55994500	1. 17445600	3. 40399600
C	-1. 84642200	0. 76052600	5. 09191200
C	-5. 09446100	0. 31579200	1. 20996900
H	-3. 95087200	-1. 47249200	1. 23712100
C	-4. 58386300	2. 00776900	2. 85329300
C	-2. 84101700	1. 56943600	4. 53514400
C	-5. 32905200	1. 59829700	1. 78149700
H	-5. 70111600	-0. 01906100	0. 37551000
H	-4. 75891100	2. 97751800	3. 31326600
H	-3. 07113200	2. 52523500	5. 00219900
H	-6. 08964200	2. 24629800	1. 35639200
C	1. 62984200	1. 60277400	-4. 10854800
H	0. 75389300	2. 17477700	-4. 40246100
C	1. 48477400	0. 31754700	-3. 65377600
H	0. 49708300	-0. 12002500	-3. 57578000
C	2. 92089000	2. 19998900	-4. 20465700
H	3. 01790800	3. 21360300	-4. 58476100
C	4. 03078100	1. 49029200	-3. 82866300
H	5. 02303400	1. 92970000	-3. 90464100
C	0. 20527700	-0. 84437300	6. 16186400
H	1. 01837500	-1. 44252500	6. 56234500
C	-0. 13654900	0. 38691500	6. 78856800
H	0. 40125100	0. 70742100	7. 67680900
C	-1. 12995600	1. 16712300	6. 26170600
H	-1. 39544500	2. 11631500	6. 72174500
C	-0. 46341700	-1. 27569100	5. 04547100
H	-0. 16603600	-2. 20303900	4. 57155500
N	1. 21799400	-0. 69011700	1. 53157600
S	2. 15189800	-1. 62841300	2. 48591600
C	3. 66869500	-2. 04833800	1. 43574000
O	1. 54998800	-2. 92304700	2. 81136200

O	2.67073900	-0.76036300	3.54816400
F	3.86606900	-1.11803400	0.49427700
F	4.73345400	-2.08867800	2.23945100
F	3.51147800	-3.23592400	0.85900700
H	-0.02132300	3.35769100	1.70935500
C	3.97044800	4.67357400	0.27003700
C	4.68885800	4.72955900	-0.93850600
C	4.29434600	5.61525200	1.25587600
C	5.67496100	5.69042400	-1.15421100
H	4.48292600	4.01212500	-1.72766800
C	5.28509900	6.57754600	1.04484100
H	3.78464200	5.61178400	2.21283700
C	5.97909200	6.62316100	-0.16161500
H	6.20682300	5.70805100	-2.10191600
H	5.51104300	7.29079000	1.83299100
H	6.74822300	7.37244200	-0.32701600
C	4.48501300	1.84077900	1.49198600
H	4.04864100	1.42641500	2.40028000
C	5.80927400	1.98915400	1.43152600
H	6.30497400	2.37821400	0.54498000
H	6.44908000	1.72225000	2.26846800

TS-1-1-3SS

l imaginary frequency

H = -5236.771551

G = -5236.963329

E(M06-2X-DCM) = -5237.924831

C	1.79921400	4.61312800	-0.63520100
C	0.89036900	4.75973500	0.63635300
H	1.45459900	5.30119800	1.40444500
H	0.02772500	5.36998900	0.35119700
C	0.39543600	3.49917200	1.26932700
C	0.89870000	3.99126400	-1.73722500
H	1.50117100	3.65352000	-2.58662700
H	0.23140700	4.77090800	-2.10489000
N	0.03688200	2.90179300	-1.29242900
C	-1.33723900	2.92170400	-1.51344700
N	-1.86658400	1.66477100	-1.47250600
C	-3.15839600	1.15492800	-1.67719100
C	-4.32750000	1.90812700	-1.86041400
C	-3.24412400	-0.24965700	-1.70126900
C	-5.54119400	1.25187100	-2.07298200
C	-4.46286500	-0.88111600	-1.92106500
H	-2.34991900	-0.84347700	-1.54284200

C	-5.62796700	-0.13823400	-2.11530400
H	-6.57553800	-0.62975700	-2.29923000
C	-4.53236800	-2.38236200	-1.86662800
C	-6.80470900	2.06541400	-2.18446200
F	-3.40445600	-2.96429800	-2.33508600
F	-5.56884000	-2.87197500	-2.57635300
F	-4.68956600	-2.82895000	-0.58889000
F	-6.57846800	3.30079500	-2.67112400
F	-7.39848700	2.22134300	-0.97230400
F	-7.71562600	1.46921000	-2.98548400
S	-2.19291300	4.35550500	-1.74177900
H	-4.28289500	2.98699200	-1.84462000
C	1.13447300	2.62645700	2.07135500
H	-1.17902700	0.92715900	-1.27534600
H	0.55330500	2.20394300	2.89714900
H	0.45937100	1.97165800	-1.26384300
H	1.31246300	1.46503000	1.56807500
O	-0.77229500	-1.29973300	0.98787800
O	1.47910400	-2.14397500	-0.02710100
P	0.64703200	-0.80099600	0.35046300
O	0.27866400	0.04449000	-0.82791500
C	-0.78443000	-3.77033600	4.37506600
C	-0.47405300	-4.29026000	3.12393800
C	-0.57614500	-3.49521100	1.97212300
C	-1.23928900	-1.59342100	3.35406000
C	-1.20922800	-2.44687700	4.47017000
C	0.94251000	-2.98943200	-1.01594900
C	-0.01126700	-3.93170800	-0.64018700
C	-0.65050800	-4.68669900	-1.63720300
C	-0.27848300	-4.56384600	-2.97099200
C	0.74081800	-3.67599300	-3.31148500
C	1.36310900	-2.85855600	-2.35342100
H	-1.50726800	-2.04295400	5.43294900
H	1.05826000	-3.58609300	-4.34624300
C	-0.47872500	-4.38823500	0.73720900
C	0.42389300	-5.53676200	1.29679600
H	0.32954600	-6.46062100	0.71736800
H	1.47051100	-5.21490600	1.25241800
H	-2.66113700	-5.51552100	-1.61887800
H	-1.42163400	-6.60846300	-1.00109600
C	-0.85262900	-2.13658200	2.11242300
H	-0.71765500	-4.38794700	5.26696700
H	-0.77202700	-5.15050700	-3.74141700
C	-0.01345100	-5.68771100	2.77030800

H	-0.82862300	-6.41701600	2.87587300
H	0.80168100	-6.03069500	3.41736800
C	-1.73311600	-5.55534000	-1.03911700
C	-1.89439700	-4.95758200	0.37339400
H	-2.25349600	-5.67841300	1.11381400
H	-2.61272300	-4.13220600	0.33533900
C	2.45239700	-1.93395800	-2.80371100
C	3.80302200	-2.26760700	-2.53974000
C	2.13884400	-0.79656500	-3.58613700
C	4.18320000	-3.42994400	-1.79562500
C	4.86031400	-1.43003100	-3.05945700
C	3.20606200	0.03168200	-4.10163100
C	5.49998600	-3.72983700	-1.56376600
H	3.40766500	-4.08187900	-1.41009900
C	6.22184100	-1.77688700	-2.79229600
C	4.53396500	-0.30664600	-3.82524800
C	6.53681100	-2.89188300	-2.06373700
H	5.75890200	-4.61700200	-0.99242700
H	7.00398900	-1.13347000	-3.18865000
H	5.33392500	0.31380900	-4.22498500
H	7.57515400	-3.14557800	-1.86862000
C	-1.73614000	-0.19229200	3.53370400
C	-2.96730000	0.19780500	2.94660000
C	-1.04202500	0.70450000	4.38618700
C	-3.76507900	-0.68346700	2.14863300
C	-3.48357400	1.52855700	3.18213500
C	-1.58858700	2.02125500	4.63845500
C	-4.95385700	-0.27528600	1.60283100
H	-3.42438900	-1.69872800	1.98299300
C	-4.71556600	1.92277200	2.57164800
C	-2.78226500	2.40101300	4.01863500
C	-5.43255600	1.05104500	1.79843400
H	-5.53134600	-0.97163200	1.00412400
H	-5.07200300	2.93588000	2.74220500
H	-3.18558700	3.39439900	4.20611900
H	-6.35591700	1.36611000	1.32198000
C	0.52245800	0.69005200	-4.66245000
H	-0.50775300	0.95510400	-4.88399200
C	0.79347300	-0.41590600	-3.89969100
H	-0.01994200	-1.01725300	-3.51247800
C	1.57865700	1.50236600	-5.16825500
H	1.34459100	2.37164500	-5.77695600
C	2.88066900	1.17954800	-4.89243400
H	3.69683700	1.78704200	-5.27677500

C	0.84977200	1.26548000	5.83182000
H	1.80521000	0.99298700	6.26991100
C	0.29211000	2.54775400	6.09847500
H	0.81332600	3.23538200	6.75909900
C	-0.88998700	2.91312100	5.51233800
H	-1.32388900	3.89296300	5.69893600
C	0.20686600	0.37608500	5.00936000
H	0.66118500	-0.58566300	4.80420300
N	1.59291400	-0.00385800	1.42076800
S	2.69554800	-0.59449600	2.47577400
C	4.14075100	-1.20154000	1.40823600
O	2.23983700	-1.79306000	3.18548500
O	3.22126200	0.55141000	3.21949100
F	4.07734200	-2.52442200	1.26650200
F	4.12408400	-0.62510900	0.20451100
F	5.27982700	-0.88392600	2.02943900
H	-0.67892100	3.33082500	1.21737900
H	2.15420000	2.90518900	2.32887100
C	3.08793200	3.82889800	-0.33493200
C	3.89683500	4.19541100	0.75669500
C	3.53854500	2.77484700	-1.14169900
C	5.09212200	3.53603100	1.03468300
H	3.59882200	5.01261900	1.40451000
C	4.74053400	2.11563600	-0.87071700
H	2.96197600	2.43665900	-1.99568200
C	5.52189200	2.48886300	0.21912000
H	5.68439000	3.84024700	1.89336300
H	5.04613900	1.29258900	-1.50836000
H	6.44692900	1.96361700	0.43931700
C	2.16018600	6.04660000	-1.17641900
H	2.73682300	5.90884000	-2.09950700
H	1.21296700	6.52661600	-1.46320800
C	2.89933200	6.99410300	-0.27233300
H	2.37777400	7.30870700	0.63302500
C	4.09863700	7.51618300	-0.53283500
H	4.65738500	7.24647300	-1.42645100
H	4.56819400	8.23264600	0.13578500

TS-1-2-3RR

l imaginary frequency

H = -5236.769005

G = -5236.964364

E(M06-2X-DCM) = -5237.611984

O	1.53413100	-1.67464400	1.40915600
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O	3.36407700	-0.40888200	0.08387000
P	1.75961900	-0.58671600	0.23259500
O	1.21782500	0.79947100	0.59721900
N	1.21753000	-1.25977400	-1.11888800
S	-0.33013700	-1.36659000	-1.45451500
C	-0.54158900	-3.19096200	-1.78950300
F	-1.82906000	-3.43118300	-2.05504100
F	-0.17238900	-3.89980800	-0.72188600
F	0.19813300	-3.56421200	-2.84018500
C	-0.49214600	4.49143000	0.04103400
C	-0.67515900	4.04040200	-1.45455100
H	-0.13875900	4.75972800	-2.08782800
H	-1.73806200	4.10546100	-1.69855900
C	-0.17136000	2.68115000	-1.80361800
C	-1.22806700	3.45241700	0.96625800
H	-0.58605300	3.11418600	1.77480000
H	-2.08037000	3.94678000	1.43073400
N	-1.72274300	2.24045300	0.30327800
C	-3.05527800	2.07551900	-0.04805900
N	-3.35029800	0.77772500	-0.34801300
C	-4.55692700	0.12650100	-0.67529800
C	-5.74782400	0.75281200	-1.06938100
C	-4.51978300	-1.27792500	-0.59976400
C	-6.87173300	-0.02413300	-1.35900800
C	-5.65447300	-2.03052600	-0.88342800
H	-3.60010200	-1.77654800	-0.31489400
C	-6.84645100	-1.41362700	-1.26490000
H	-7.72981200	-2.00075000	-1.48321200
C	-5.60541000	-3.52267400	-0.69175200
C	-8.12165500	0.66215900	-1.84811800
F	-4.40088100	-4.03931500	-1.01292900
F	-5.83868800	-3.86245500	0.60603600
F	-6.53642900	-4.16119400	-1.43112600
F	-9.23161500	-0.05735800	-1.56619500
F	-8.27807800	1.88316300	-1.29557800
F	-8.09817000	0.83691600	-3.19026900
S	-4.12650700	3.37465400	-0.11216800
H	-5.79816900	1.82920700	-1.13546600
C	1.13456000	2.22266200	-1.67148300
H	-2.56666000	0.11968700	-0.28652200
H	1.92918800	2.94333900	-1.48832200
H	1.39736400	1.36649700	-2.29652300
O	-1.21172100	-1.11649600	-0.27787900
H	-1.21655400	1.39210900	0.54999100

O	-0.69373500	-0.68152300	-2.70178500
H	1.09457200	1.59107600	-0.53744900
C	5.42064600	-3.74731800	-1.38348700
C	5.06590300	-3.67421100	-0.04092700
C	4.47261300	-2.51325800	0.48165500
C	4.52055300	-1.50159300	-1.74388100
C	5.18398100	-2.64838200	-2.20988200
C	2.07563900	-1.54892600	2.69273400
C	3.40901200	-1.89646500	2.90011800
C	3.97728400	-1.67156600	4.16450100
C	3.19535100	-1.23146000	5.22708100
C	1.83590500	-1.00208700	5.02026100
C	1.24518200	-1.13116600	3.75090700
H	5.49308200	-2.67687400	-3.25046000
H	1.20780100	-0.69452900	5.85071700
C	4.42149600	-2.60755800	2.00444600
C	4.33941100	-4.16191200	2.17851500
H	3.29877000	-4.47737300	2.04135000
H	4.65889300	-4.48844200	3.17280600
H	5.67916100	-2.91821600	4.66703000
H	6.05256400	-1.19860200	4.63984400
C	4.12815600	-1.48603600	-0.39221100
H	5.88670800	-4.64258600	-1.78705600
H	3.63091700	-1.07800600	6.21118200
C	5.21216800	-4.72703900	1.03639000
H	4.87919400	-5.71571100	0.70095900
H	6.25989500	-4.83754800	1.34880800
C	5.45893700	-1.97622500	4.14578600
C	5.75715600	-2.08447200	2.63560400
H	5.97280300	-1.08998700	2.22792400
H	6.60905100	-2.73093300	2.40469900
C	-0.21333000	-0.85006600	3.58087400
C	-0.72016000	0.43796700	3.89235800
C	-1.09694600	-1.88327400	3.17659200
C	0.11398300	1.53633400	4.28671000
C	-2.14276800	0.68509800	3.80832400
C	-2.50937300	-1.60477300	3.04812500
C	-0.41721700	2.75513000	4.62596200
H	1.18796100	1.39428400	4.31674800
C	-2.65542200	1.97202300	4.16724700
C	-2.99372500	-0.33550700	3.37511700
C	-1.82299900	2.97798000	4.57775800
H	0.24223800	3.56513300	4.92642100
H	-3.72862000	2.13273600	4.10157500

H	-4.06064800	-0.13795800	3.29577100
H	-2.22467200	3.95096500	4.84549800
C	4.30486500	-0.34446300	-2.66817200
C	3.46628400	-0.48379300	-3.80188400
C	5.01563100	0.86367100	-2.45050100
C	2.69969500	-1.66553600	-4.06243700
C	3.34672600	0.61103300	-4.73997900
C	4.86597200	1.95742400	-3.38412100
C	1.90400700	-1.76797400	-5.17275100
H	2.72669600	-2.47544000	-3.34474200
C	2.51295100	0.45757400	-5.89229400
C	4.04214000	1.79940400	-4.50221100
C	1.81547400	-0.69908600	-6.10907000
H	1.31554000	-2.66701800	-5.33008700
H	2.44412800	1.28811900	-6.59104400
H	3.94539400	2.62086600	-5.20961900
H	1.18063000	-0.80211100	-6.98477200
C	-1.54003300	-4.18229700	2.47297800
H	-1.17772500	-5.18491600	2.26258900
C	-0.66393000	-3.21984600	2.90140600
H	0.38097700	-3.47284500	3.03716900
C	-2.92172800	-3.88750800	2.29983600
H	-3.60119200	-4.65143100	1.93512900
C	-3.39066000	-2.63633900	2.59510000
H	-4.44577700	-2.40393200	2.47996100
C	6.58628000	2.23558400	-1.17208600
H	7.26385100	2.34765900	-0.32974700
C	6.41401900	3.31756100	-2.08107500
H	6.95469700	4.24676900	-1.92269500
C	5.58007600	3.17567400	-3.15672100
H	5.44894000	3.98754000	-3.86846500
C	5.91450300	1.05466800	-1.35172800
H	6.07120700	0.23953500	-0.65461600
C	-1.24007500	5.86467100	0.17891400
H	-0.83026000	6.56546700	-0.56071100
H	-2.29123200	5.70096400	-0.07890400
H	-0.88617200	1.98405900	-2.23914800
C	-1.14498600	6.48618700	1.54657800
H	-0.14372400	6.74106200	1.89339600
C	-2.19341500	6.74569400	2.33080500
H	-3.20993300	6.50768100	2.02473300
H	-2.07431100	7.21443300	3.30452100
C	1.00837000	4.70125700	0.35759800
C	1.71987900	5.67864800	-0.36678000

C	1. 72388100	3. 98102200	1. 32405500
C	3. 07298400	5. 92063200	-0. 14322400
H	1. 21387100	6. 26664200	-1. 12771000
C	3. 08294300	4. 22044600	1. 55164400
H	1. 25242800	3. 19768800	1. 90322400
C	3. 76638400	5. 18914600	0. 82314100
H	3. 58512200	6. 68082100	-0. 72725800
H	3. 60427500	3. 63068700	2. 30068200
H	4. 82320900	5. 36970200	0. 99808000

TS-1-2-3SR

l imaginary frequency

H = -5236. 765193

G = -5236. 959972

E(M06-2X-DCM) = -5237. 611281

O	-2. 22130500	0. 47206400	1. 73775100
O	-3. 31195200	-1. 03113300	-0. 08071700
P	-2. 00518600	-0. 12301900	0. 24502100
O	-1. 93227100	1. 11798700	-0. 64119700
N	-0. 72004300	-1. 08785600	0. 29705600
S	-0. 24999400	-2. 08809700	-0. 85599100
C	-0. 85033400	-3. 76881500	-0. 29234700
F	-0. 49955700	-4. 68173800	-1. 19948300
F	-0. 30072400	-4. 09182300	0. 88459400
F	-2. 17898600	-3. 76219300	-0. 16185500
C	0. 94857100	3. 79318900	-1. 01123900
C	1. 31780800	3. 08552100	-2. 37300100
H	0. 92721300	3. 71264700	-3. 18363300
H	2. 40670500	3. 06107100	-2. 44790800
C	0. 79279400	1. 70528400	-2. 59311700
C	1. 16828400	2. 78203000	0. 18158500
H	0. 21491100	2. 61121800	0. 68425500
H	1. 86111300	3. 20437500	0. 90745500
N	1. 66612300	1. 45735900	-0. 20343500
C	3. 02424000	1. 16795400	-0. 28961900
N	3. 25150400	-0. 15803500	-0. 53230500
C	4. 46347400	-0. 87277900	-0. 65819700
C	5. 66437100	-0. 32612700	-1. 12979000
C	4. 41314100	-2. 23857100	-0. 33833600
C	6. 79500400	-1. 13771700	-1. 24063600
C	5. 55348200	-3. 02906400	-0. 45036700
H	3. 47900700	-2. 67664500	-0. 00713300
C	6. 75882700	-2. 48761400	-0. 89725900
H	7. 64245300	-3. 10677300	-0. 99102600

C	5.49362300	-4.46389500	-0.00090700
C	8.09190700	-0.52058100	-1.69685100
F	6.43557600	-5.22353000	-0.59864700
F	4.29299600	-5.02605200	-0.25061200
F	5.70068500	-4.56961800	1.33953400
F	8.90401000	-1.43253000	-2.27774300
F	8.77969000	0.01536000	-0.66271500
F	7.89083500	0.47132700	-2.59143600
S	4.19136500	2.36525300	-0.15502600
H	5.71625000	0.71611200	-1.40647200
C	-0.52824500	1.36139300	-2.86416700
H	2.43475800	-0.77717600	-0.52689500
H	-1.19862800	2.15220300	-3.20397600
H	-0.69872200	0.37707200	-3.30094700
O	1.22264300	-2.20517000	-0.80368900
H	1.06644800	0.68208200	0.07862000
O	-0.87150300	-1.86870900	-2.17038600
H	-1.09089500	1.17181400	-1.71552500
C	-6.99889300	0.96020700	-0.25025700
C	-6.45913900	0.56895000	0.97005700
C	-5.26812800	-0.17216100	1.01937900
C	-5.09713800	-0.05208300	-1.41538100
C	-6.33389000	0.61682200	-1.42661600
C	-2.40490500	-0.39204200	2.83146900
C	-3.65874700	-0.96466600	3.04615800
C	-3.79776600	-1.93745900	4.05014600
C	-2.73954900	-2.24129700	4.89848600
C	-1.53137400	-1.56616200	4.73985900
C	-1.32500100	-0.64301500	3.69992100
H	-6.75945900	0.89142000	-2.38705400
H	-0.70698500	-1.76636800	5.41725200
C	-5.02896300	-0.66639100	2.44092000
C	-5.77022000	0.45246600	3.24911700
H	-6.05194700	0.12442700	4.25414800
H	-5.10005400	1.31344400	3.35461300
H	-5.16965500	-3.63070600	4.10240900
H	-5.79147300	-2.17424300	4.87054900
C	-4.56980800	-0.41115000	-0.16082500
H	-7.92918600	1.52085200	-0.29333400
H	-2.85086300	-2.98610900	5.68231700
C	-6.97765500	0.83561500	2.36623000
H	-7.85387600	0.21219000	2.59230200
H	-7.28962500	1.87695400	2.50507200
C	-5.18615200	-2.53748300	4.02834300

C	-5.74202100	-2.04029900	2.67814900
H	-6.83256000	-1.95277800	2.66006400
H	-5.44858100	-2.73101500	1.87931100
C	0.00360800	0.03934800	3.60977200
C	0.10779100	1.42524600	3.88900100
C	1.17184100	-0.73036400	3.38039000
C	-1.02386600	2.24855700	4.19528600
C	1.41133700	2.05137500	3.91120300
C	2.46981100	-0.09656400	3.44261000
C	-0.88472700	3.58419200	4.46918800
H	-2.00912400	1.79723600	4.22172400
C	1.51188900	3.45147600	4.18988900
C	2.55339200	1.27631700	3.69127000
C	0.39859000	4.20145100	4.45858800
H	-1.76221400	4.18055900	4.70458900
H	2.50140000	3.90241900	4.19653400
H	3.53142800	1.75110700	3.72104200
H	0.48878800	5.26174100	4.67856200
C	-4.42310600	-0.36195000	-2.71311900
C	-4.26028800	-1.70773100	-3.12609700
C	-4.02728100	0.69859000	-3.56718100
C	-4.68354400	-2.82284300	-2.33461700
C	-3.66922600	-1.99182800	-4.41380000
C	-3.47158700	0.39745200	-4.86784800
C	-4.50353700	-4.11191200	-2.76228100
H	-5.16133300	-2.63884300	-1.37942400
C	-3.49461600	-3.35113600	-4.82083700
C	-3.29918600	-0.93563300	-5.24985000
C	-3.89356300	-4.38511800	-4.01911800
H	-4.83221500	-4.93798300	-2.13746700
H	-3.03673900	-3.54284100	-5.78818700
H	-2.87136000	-1.15690500	-6.22557200
H	-3.75405100	-5.41426900	-4.33808800
C	2.28395800	-2.85251300	2.90003100
H	2.22245000	-3.91004300	2.65830900
C	1.13322100	-2.12947300	3.07668100
H	0.17247200	-2.61409300	2.96127000
C	3.56168500	-2.23167200	3.00420400
H	4.45836100	-2.82443500	2.85187900
C	3.64628100	-0.88824800	3.25358200
H	4.61245300	-0.39305100	3.30875500
C	-3.77320900	3.08198700	-4.06490900
H	-3.87307300	4.12000800	-3.75857600
C	-3.25928000	2.77778400	-5.35857300

H	-2.98425800	3.58380900	-6.03357600
C	-3.10541400	1.47165700	-5.73911700
H	-2.70111500	1.22303000	-6.71763300
C	-4.13646800	2.08053600	-3.20047800
H	-4.50250300	2.33267700	-2.21247400
C	-0.56305600	4.22844800	-1.07239400
H	-0.67453900	4.87150300	-1.95726500
H	-1.18365000	3.34397500	-1.22681200
C	-1.09595000	4.96440200	0.12893000
C	-2.01698900	4.46915400	0.95885000
H	-2.38447800	5.04439000	1.80466700
H	-2.43122400	3.47239800	0.82686600
C	1.79910500	5.07254600	-0.85818500
C	2.32986900	5.75325100	-1.96431300
C	1.99122800	5.65580600	0.40675300
C	3.03972400	6.94653400	-1.81657600
H	2.20859900	5.35772000	-2.96711700
C	2.69779700	6.84843600	0.55801900
H	1.58016900	5.18508700	1.29395800
C	3.23091300	7.50122800	-0.55319100
H	3.44553100	7.43770600	-2.69716800
H	2.83238100	7.26517200	1.55285300
H	3.78629600	8.42763500	-0.43545200
H	-0.70573300	5.96596500	0.30041900
H	1.52956900	0.90655700	-2.62416300

TS-1-2-3SS

l imaginary frequency

H = -5236.765781

G = -5236.961573

E(M06-2X-DCM) = -5237.610270

O	-2.03852800	0.30917300	1.87183700
O	-3.00462300	-1.32717700	0.10079700
P	-1.83876300	-0.21874300	0.35002900
O	-2.01289200	1.02504600	-0.50291100
N	-0.41879800	-0.98693900	0.29714200
S	0.07494400	-1.92075300	-0.89870000
C	-0.24407100	-3.66846200	-0.30791900
F	0.14014300	-4.52470900	-1.25628700
F	0.45421200	-3.91365600	0.80783400
F	-1.54184200	-3.84479700	-0.05235900
C	0.63445800	3.97405400	-1.11203900
C	1.05523500	3.28849700	-2.46816900
H	0.68902200	3.90626800	-3.29616300

H	2.14629700	3.29137300	-2.51097000
C	0.55876500	1.90162600	-2.68165200
C	1.00733500	2.99041100	0.06366600
H	0.10713200	2.66021800	0.57631400
H	1.63414400	3.51168800	0.78902800
N	1.66596000	1.74223300	-0.34618600
C	3.04559700	1.58976900	-0.43618100
N	3.39803900	0.29806900	-0.69415000
C	4.67159800	-0.29880100	-0.82757300
C	5.80697700	0.35370200	-1.32459100
C	4.75462200	-1.65899300	-0.49189100
C	7.00788600	-0.34815400	-1.44540800
C	5.96283200	-2.33932900	-0.61443500
H	3.87093800	-2.17787800	-0.13914400
C	7.10418700	-1.69122500	-1.08718600
H	8.04091400	-2.22530800	-1.18917200
C	6.04971500	-3.76738700	-0.14755800
C	8.23307600	0.38328200	-1.92992400
F	6.32176000	-3.83459600	1.18348200
F	7.03041200	-4.44814900	-0.77730600
F	4.89499000	-4.43737800	-0.33969300
F	8.88190600	0.99621400	-0.91360000
F	7.92413900	1.33992300	-2.83253200
F	9.11929600	-0.45450600	-2.51340600
S	4.11089300	2.87944400	-0.27276000
C	1.49525000	5.28745700	-1.01652900
H	2.55140600	5.00844900	-1.04576000
H	1.28143900	5.88631100	-1.91333100
H	5.75546500	1.39224900	-1.61504100
C	-0.78045100	1.52470100	-2.80806000
H	2.64076900	-0.39440300	-0.70413600
H	-1.49912600	2.31111700	-3.04326400
H	-0.96015300	0.55884800	-3.28305000
O	1.55222800	-1.85547600	-0.96977500
H	1.15801000	0.90189900	-0.06726100
O	-0.66748600	-1.77985300	-2.16023700
H	-1.20668800	1.25908300	-1.66235400
C	-6.93344300	0.13205900	0.09899900
C	-6.28442800	-0.15551600	1.29488900
C	-5.00582200	-0.73392800	1.29121300
C	-4.98264200	-0.66346900	-1.15043000
C	-6.29479200	-0.16032900	-1.10578100
C	-2.05270300	-0.57674100	2.95818500
C	-3.21299200	-1.29842100	3.23841500

C	-3.17791900	-2.27542700	4.24703400
C	-2.04595800	-2.44443400	5.03598000
C	-0.93912000	-1.62836000	4.81318600
C	-0.90527300	-0.69028400	3.76668400
H	-6.80572000	0.02344800	-2.04610300
H	-0.06164900	-1.72281200	5.44539100
C	-4.63764100	-1.17405400	2.70295000
C	-5.47212100	-0.14501200	3.53807500
H	-5.66157600	-0.49093900	4.55874300
H	-4.91040600	0.79408900	3.60262800
H	-4.33272400	-4.12018000	4.37832300
H	-5.08199800	-2.74064000	5.17448700
C	-4.34174100	-0.90331200	0.07950700
H	-7.92964400	0.56724000	0.09667700
H	-2.02363600	-3.19287100	5.82396400
C	-6.76035200	0.07168500	2.71352300
H	-7.54144900	-0.64895300	2.99297700
H	-7.19016600	1.06980900	2.85592700
C	-4.48330300	-3.03737600	4.30191600
C	-5.16554200	-2.62239100	2.98244900
H	-6.25808000	-2.66762900	3.02209100
H	-4.83297700	-3.27982900	2.17093100
C	0.31680800	0.15642300	3.60589700
C	0.24838500	1.55273600	3.84386000
C	1.56578600	-0.45939700	3.34022700
C	-0.97116800	2.23388500	4.16259800
C	1.45862200	2.34331700	3.80005300
C	2.77161900	0.33825100	3.34193700
C	-1.00024900	3.58722800	4.38102800
H	-1.88755000	1.66085300	4.24212500
C	1.38374700	3.75383100	4.02776700
C	2.68445800	1.71598400	3.55955500
C	0.19065000	4.36424000	4.30458700
H	-1.94122800	4.07372000	4.62457900
H	2.30379200	4.33053900	3.97669300
H	3.59275300	2.31383700	3.54251400
H	0.14751800	5.43625200	4.47574500
C	-4.35428800	-0.95262400	-2.47589400
C	-4.05555100	-2.28969500	-2.84004600
C	-4.14808300	0.10034800	-3.40211500
C	-4.28782300	-3.40529400	-1.97373500
C	-3.51925100	-2.56846500	-4.15260700
C	-3.64755000	-0.20061100	-4.72532700
C	-3.98067400	-4.68455100	-2.35653600

H	-4. 72137600	-3. 23062800	-0. 99599700
C	-3. 20696800	-3. 91659800	-4. 51145700
C	-3. 33735100	-1. 52135200	-5. 05895000
C	-3. 42425600	-4. 94824600	-3. 63982200
H	-4. 16562600	-5. 51023800	-1. 67466400
H	-2. 79275300	-4. 10200900	-5. 49955400
H	-2. 95119200	-1. 74119400	-6. 05225400
H	-3. 18149700	-5. 96870600	-3. 92300200
C	2. 92578700	-2. 42752100	2. 84042900
H	2. 99449200	-3. 48746200	2. 61104600
C	1. 69792700	-1. 85648900	3. 05190800
H	0. 80439100	-2. 46255200	2. 97479600
C	4. 11525600	-1. 64543400	2. 89232200
H	5. 07511600	-2. 12073000	2. 71585000
C	4. 03371900	-0. 29839000	3. 12143900
H	4. 92867700	0. 31859600	3. 13350200
C	-4. 22918000	2. 46544900	-4. 02416000
H	-4. 42525600	3. 49881000	-3. 75286100
C	-3. 77261300	2. 15665900	-5. 33778900
H	-3. 64804600	2. 95263700	-6. 06727400
C	-3. 48017700	0. 86123800	-5. 66948100
H	-3. 11534800	0. 61108000	-6. 66308100
C	-4. 40243800	1. 47620100	-3. 08997800
H	-4. 71870200	1. 73654100	-2. 08700400
C	-0. 85101400	4. 40863500	-1. 11276900
C	-1. 36492600	5. 11247900	-2. 21874700
C	-1. 70232100	4. 25423900	-0. 00830700
C	-2. 66640900	5. 61040800	-2. 23569500
H	-0. 74042600	5. 29560800	-3. 08892800
C	-3. 00864800	4. 75079000	-0. 02066000
H	-1. 36837700	3. 75506500	0. 89292300
C	-3. 50210200	5. 42791700	-1. 13250700
H	-3. 02192200	6. 14881900	-3. 11056300
H	-3. 63704400	4. 60281900	0. 85321600
H	-4. 51711600	5. 81572200	-1. 13878400
C	1. 23331500	6. 12866100	0. 20332300
C	2. 15459600	6. 41671100	1. 12521300
H	3. 17070900	6. 03476900	1. 05668300
H	1. 92619300	7. 05010000	1. 97874700
H	0. 22656400	6. 53010300	0. 31272500
H	1. 31150200	1. 12591800	-2. 80795900

INT-13

0 imaginary frequency

H = -5315.396272

G = -5315.600145

E(M06-2X-DCM) = -5316.278567

E(M06-2X-cyclohexane) = -5316.253995

C	-2.94506900	3.94204900	-0.54302300
C	-3.96102900	3.43762400	0.52439000
H	-3.60520700	2.46605300	0.89403400
H	-3.94699500	4.12349600	1.37875400
C	-5.38362700	3.27944900	0.05210200
C	-2.88509700	2.94353700	-1.73670300
H	-2.19132000	3.31961700	-2.49920600
H	-3.86451100	2.86042500	-2.20800900
N	-2.47947800	1.60102700	-1.35230000
C	-3.11177700	0.45449400	-1.71340200
N	-2.41651800	-0.66438400	-1.30029500
C	-2.75167900	-2.02321200	-1.36910800
C	-4.06834300	-2.51225700	-1.35266200
C	-1.69016500	-2.94119300	-1.38355800
C	-4.29676000	-3.88630000	-1.38135200
C	-1.94029200	-4.31236300	-1.40370700
H	-0.66698500	-2.57981800	-1.37366200
C	-3.24460500	-4.80221700	-1.41579300
H	-3.43765300	-5.86752700	-1.45019500
C	-0.78804800	-5.27188800	-1.32743900
C	-5.70751100	-4.40279100	-1.27388300
F	0.31191900	-4.80521500	-1.96589200
F	-1.08230900	-6.47630200	-1.85569400
F	-0.41096300	-5.49616200	-0.03566100
F	-6.61479700	-3.52717400	-1.74411300
F	-6.03971300	-4.65838600	0.02074200
F	-5.86878300	-5.56446200	-1.94598300
S	-4.55376900	0.41468200	-2.59515300
H	-4.89815100	-1.82171200	-1.32531200
C	-6.42935900	3.92979100	0.57311800
H	-1.46735200	-0.48443100	-0.97106700
H	-1.55298600	1.51353100	-0.94066300
H	1.13440800	1.93373400	1.53342800
O	0.94183700	-1.41280300	1.03517500
O	2.81146500	-0.26915100	-0.33785100
P	1.36672000	-0.02922200	0.32945400
O	0.23962400	0.42772100	-0.51998000
C	3.22726600	-2.83390600	4.23831700
C	3.67686200	-2.99631800	2.93294000
C	2.86411200	-2.63656300	1.84583000

C	1. 15890300	-1. 82981300	3. 40754600
C	1. 95821100	-2. 29756300	4. 46256400
C	2. 99695800	-1. 30027900	-1. 28820300
C	3. 22774400	-2. 59853900	-0. 83947400
C	3. 31361800	-3. 62636100	-1. 79507900
C	3. 25229400	-3. 34703500	-3. 15549300
C	3. 09621900	-2. 02672300	-3. 57439900
C	2. 95053300	-0. 97449600	-2. 65679900
H	1. 58002500	-2. 20484500	5. 47623100
H	3. 06282000	-1. 79200400	-4. 63411200
C	3. 48350300	-3. 16788400	0. 55583000
C	4. 99740400	-3. 12389900	0. 94653200
H	5. 60883600	-3. 78170900	0. 32103000
H	5. 36481900	-2. 09876800	0. 82397800
H	2. 79706000	-5. 72713500	-1. 58259500
H	4. 47512900	-5. 34937900	-1. 18851100
C	1. 67108800	-1. 97371000	2. 10442400
H	3. 85097600	-3. 12441300	5. 07973100
H	3. 32069900	-4. 14745500	-3. 88739100
C	5. 01526800	-3. 50853100	2. 44431800
H	5. 10755000	-4. 59471300	2. 58037800
H	5. 85146500	-3. 05064100	2. 98407400
C	3. 44460700	-4. 97336800	-1. 12396400
C	3. 04413900	-4. 65713900	0. 32974300
H	3. 49154300	-5. 33498000	1. 06217600
H	1. 95693100	-4. 72915900	0. 42904100
C	2. 78132300	0. 42449700	-3. 16698600
C	3. 88894700	1. 30622600	-3. 15951300
C	1. 54877400	0. 82912600	-3. 73191800
C	5. 18541500	0. 91993900	-2. 69140400
C	3. 73568000	2. 64742700	-3. 67563000
C	1. 41341700	2. 16996200	-4. 25673100
C	6. 24048600	1. 79498100	-2. 70765100
H	5. 32983100	-0. 08997100	-2. 32333200
C	4. 85755700	3. 53380900	-3. 66015200
C	2. 50210400	3. 04378000	-4. 20006300
C	6. 07637700	3. 12457100	-3. 18986200
H	7. 21482900	1. 47254200	-2. 35038400
H	4. 72149200	4. 54198900	-4. 04460700
H	2. 39341600	4. 05233200	-4. 59446400
H	6. 92306100	3. 80551600	-3. 19091500
C	-0. 19219300	-1. 24224700	3. 67365200
C	-1. 35118600	-1. 94303800	3. 25311500
C	-0. 31598700	-0. 02066500	4. 38135300

C	-1.29860100	-3.21217900	2.59286900
C	-2.65827100	-1.38171700	3.51112100
C	-1.63166300	0.52302600	4.63993500
C	-2.43965500	-3.85887100	2.19600600
H	-0.33519300	-3.67331200	2.40800500
C	-3.82323100	-2.08254900	3.06692200
C	-2.76156700	-0.16564200	4.19157000
C	-3.72290600	-3.28511700	2.42148800
H	-2.36078700	-4.81636500	1.69143300
H	-4.79527900	-1.63252300	3.25393400
H	-3.74801300	0.25207400	4.38285200
H	-4.61067800	-3.79874600	2.06542200
C	-0.76280900	0.38272100	-4.39133300
H	-1.61394000	-0.28963900	-4.44414100
C	0.41071900	-0.03641900	-3.82151600
H	0.48976600	-1.04571700	-3.43331300
C	-0.89036900	1.70554800	-4.90510200
H	-1.83166100	2.01670400	-5.34877700
C	0.16775300	2.57117500	-4.83490100
H	0.08631300	3.58153200	-5.22950200
C	0.65490500	1.91120600	5.52599000
H	1.53268700	2.45804400	5.85735000
C	-0.64318600	2.43734400	5.78321000
H	-0.74815100	3.37402600	6.32389900
C	-1.75099800	1.76017600	5.34800100
H	-2.74910000	2.14855300	5.53718200
C	0.81132000	0.72835000	4.85031700
H	1.80874000	0.34843100	4.66338100
N	1.79700100	1.15407000	1.46227400
S	3.27230700	1.52308000	2.19493900
C	4.34588400	2.24050400	0.80426700
O	3.93305100	0.30225700	2.62785900
O	2.99529400	2.63889300	3.09074500
F	3.58007700	2.71483800	-0.17582400
F	5.06187800	3.23344400	1.33005500
F	5.16017000	1.29931500	0.34577400
H	-5.55959000	2.55120300	-0.74042700
H	-6.25860900	4.64441300	1.38205900
C	-1.53453100	4.11652700	0.05678000
C	-1.23422000	3.86098300	1.40279100
C	-0.48017500	4.56754100	-0.75995300
C	0.04981200	4.07599000	1.91895500
H	-2.00055400	3.50015000	2.07858700
C	0.80163700	4.77723200	-0.25704200

H	-0.65843300	4.76252700	-1.81347500
C	1.07339400	4.54389300	1.09288400
H	0.24164000	3.88631000	2.97204100
H	1.58950500	5.12257100	-0.92110300
H	2.06595900	4.71718300	1.49750000
C	-3.43023100	5.30428500	-1.14683300
H	-2.74608900	5.60374700	-1.94960600
H	-4.40472600	5.11760300	-1.61771400
C	-3.56995600	6.43609000	-0.16573800
H	-4.36644100	6.34054000	0.57301700
C	-2.81352100	7.53715900	-0.15291100
H	-2.01901300	7.63756700	-0.89486400
C	-7.85824100	3.75145800	0.14415300
H	-7.94479000	3.01922300	-0.66527900
H	-8.48565700	3.41049100	0.97925800
H	-8.29145100	4.69876000	-0.20526600
C	-2.95994200	8.67759700	0.81338000
H	-3.16240400	9.62211400	0.28988800
H	-3.77674200	8.50223700	1.52194500
H	-2.03755600	8.83082700	1.39011000

INT-13'

0 imaginary frequency

H = -5315.378086

G = -5315.584195

E(M06-2X-DCM) = -5316.274414

E(M06-2X-cyclohexane) = -5316.244824

O	-0.58011000	-2.39386600	-0.92380900
O	-2.62095500	-0.98607300	-0.16580100
P	-0.98325500	-1.02062500	-0.11915300
O	-0.48324700	0.20846800	-0.81422900
C	-1.61854500	-2.51824500	-4.98039400
C	-2.53802800	-2.87245800	-3.99843100
C	-2.15940100	-2.90589700	-2.64865700
C	0.08241000	-2.15859600	-3.25295500
C	-0.31490300	-2.20015800	-4.60171500
C	-3.35736100	-2.03858000	0.38818700
C	-3.52774200	-3.21553700	-0.34285300
C	-4.12057800	-4.32727000	0.27702300
C	-4.63733700	-4.23302000	1.56391800
C	-4.57312000	-3.00915100	2.22719100
C	-3.93118500	-1.89173500	1.66669500
H	0.42233400	-1.95701200	-5.36102700
H	-5.01244700	-2.90532800	3.21483500

C	-3.26669900	-3.53339600	-1.81294000
C	-4.51219500	-3.18522900	-2.69727400
H	-4.83102600	-2.16135900	-2.46820200
H	-5.36123900	-3.84815400	-2.50394100
H	-5.07808500	-5.75020300	-1.05099500
H	-3.75573800	-6.44121400	-0.11684400
C	-0.88436100	-2.48102300	-2.28162500
H	-1.90163200	-2.50081400	-6.02997100
H	-5.09888900	-5.09239200	2.04376300
C	-3.99377900	-3.25801900	-4.15052600
H	-4.53861500	-2.59087800	-4.82858800
H	-4.09578100	-4.27261500	-4.56069900
C	-4.08363300	-5.53328800	-0.63590900
C	-3.09831500	-5.08822100	-1.73672100
H	-2.07146000	-5.31446000	-1.42758500
H	-3.27195600	-5.57501100	-2.70156300
C	-3.96773500	-0.60462900	2.43052600
C	-3.30591000	-0.50008600	3.67790200
C	-4.78996500	0.45498200	1.97119300
C	-2.42923900	-1.51718400	4.17498100
C	-3.49804000	0.67784900	4.49352000
C	-4.95137400	1.63806300	2.78625200
C	-1.80998300	-1.39177000	5.39028000
H	-2.22436300	-2.37909900	3.55345200
C	-2.84743900	0.76016200	5.76524000
C	-4.31264600	1.71193500	4.02667900
C	-2.02943900	-0.24518000	6.20527400
H	-1.12550000	-2.16543600	5.72544000
H	-3.01821500	1.64551400	6.37380700
H	-4.45230000	2.59781700	4.64315200
H	-1.53468400	-0.16794600	7.16977100
C	1.50640300	-1.82885400	-2.93572300
C	2.03629000	-0.57076200	-3.31628600
C	2.35566200	-2.81442200	-2.37187200
C	1.22077900	0.49509200	-3.82083600
C	3.45485200	-0.32328500	-3.18849900
C	3.76140100	-2.52824500	-2.19446200
C	1.76959800	1.68581900	-4.22301600
H	0.14656300	0.35932700	-3.86262600
C	3.99154200	0.92287600	-3.64696700
C	4.27628000	-1.30149300	-2.62216000
C	3.17650800	1.89978700	-4.15540200
H	1.12059600	2.47404200	-4.59374800
H	5.06713000	1.07164500	-3.58261800

H	5.33903900	-1.10069000	-2.50597100
H	3.59766400	2.83888100	-4.50563000
C	-6.30155300	1.44501300	0.31967500
H	-6.83619900	1.37522900	-0.62387300
C	-5.51214200	0.40346000	0.73468600
H	-5.43569100	-0.48691600	0.12103800
C	-6.43789700	2.61712300	1.11726900
H	-7.07360300	3.43040300	0.77683600
C	-5.78254500	2.70346300	2.31679600
H	-5.88914800	3.58513700	2.94486400
C	2.74096900	-5.03832800	-1.43322300
H	2.35878600	-6.01340200	-1.14340300
C	4.11832000	-4.73933200	-1.23481600
H	4.77330300	-5.48413000	-0.79098100
C	4.61080800	-3.52011200	-1.61222800
H	5.66333800	-3.28080400	-1.47982400
C	1.89466700	-4.11374700	-1.98644800
H	0.85236700	-4.36755800	-2.13717200
C	-1.69792600	3.82822700	-0.90637100
C	-2.20508100	3.06129600	0.35403400
H	-3.30011200	3.02122800	0.31244300
H	-1.86578300	2.02350400	0.30607900
C	-1.77649800	3.65139000	1.67439500
C	-0.16193100	4.01015000	-0.80117000
H	0.03929900	4.65388500	0.06052800
H	0.22550300	4.50604900	-1.69813800
N	0.57812800	2.75310200	-0.59947800
C	1.81177100	2.71028000	-0.13258700
N	2.41279100	1.54920600	0.15828100
C	3.76245000	1.37769400	0.60443300
C	4.82015900	1.60343200	-0.27589900
C	4.00092600	0.91932100	1.90492100
C	6.13153900	1.38695000	0.15361200
C	5.31635500	0.70411200	2.31557200
H	3.16812600	0.71976300	2.57170000
C	6.38560600	0.93792300	1.44735300
H	7.40341700	0.77398900	1.77915200
C	5.58266400	0.16704800	3.70159700
C	7.25211300	1.62753000	-0.82354100
F	4.68859300	0.63601500	4.59349100
F	6.81617000	0.51583400	4.13484700
F	5.51651900	-1.17863900	3.73045900
F	8.46464800	1.44129600	-0.27027800
F	7.21238400	2.88648100	-1.31498400

F	7.16326300	0.79556300	-1.89290200
S	2.62740400	4.26971800	0.10890500
H	4.61312300	1.92464200	-1.29120100
H	1.86040600	0.67541400	0.15288900
H	0.10648800	1.84376500	-0.77546700
C	-1.01946200	3.01795900	2.57768900
H	-0.67496300	2.00364400	2.36943300
H	3.72068600	3.74556400	0.69483900
N	-0.60719800	-1.29632000	1.42735700
S	0.88758500	-1.30896900	1.94468400
O	1.06676000	-0.53015300	3.18000700
O	1.90320600	-1.08852400	0.87677800
C	1.14703000	-3.08696500	2.45462200
F	0.27301700	-3.42643300	3.41386900
F	2.38688900	-3.23619000	2.93283400
F	0.97973900	-3.90110500	1.41021900
C	-2.06857400	3.12043100	-2.22533100
C	-2.84495600	1.95585300	-2.26904300
C	-1.64423400	3.66440400	-3.45102300
C	-3.17505500	1.35469300	-3.48679900
H	-3.19352700	1.48990000	-1.35648000
C	-1.97444100	3.07043800	-4.66800200
H	-1.05100800	4.57552800	-3.46807400
C	-2.74298300	1.90460800	-4.69134900
H	-3.76591700	0.44291100	-3.48363000
H	-1.63388700	3.52105500	-5.59704400
H	-2.99943700	1.43391100	-5.63666100
C	-2.28177000	5.28671100	-0.92707100
H	-1.94164200	5.79885500	-0.01588800
H	-1.84188900	5.83615900	-1.76799700
C	-3.78141900	5.37565200	-1.01427200
C	-4.45069900	5.92183600	-2.03304200
H	-3.88754500	6.32428400	-2.87719100
H	-4.34668800	4.97178700	-0.17375100
H	-2.14148800	4.65188500	1.91562600
C	-0.61913100	3.57598200	3.91287100
H	0.47387000	3.61960100	4.01459700
H	-1.01695600	4.58523800	4.06905000
H	-0.97890900	2.93041600	4.72412600
C	-5.94534900	6.03093100	-2.12648400
H	-6.32505200	5.50926600	-3.01537500
H	-6.43544100	5.60086300	-1.24633400
H	-6.26554300	7.07801600	-2.21652600

INT-13' -1

0 imaginary frequency

H = -5315.379142

G = -5315.585391

E(M06-2X-DCM) = -5316.274056

E(M06-2X-cyclohexane) = -5316.244671

O	-0.53091400	-2.56243300	-0.28177900
O	-2.61788100	-1.05245700	0.01697300
P	-0.98247500	-1.03199200	0.10779900
O	-0.48616000	-0.02627100	-0.88534900
C	-1.45254000	-3.81418700	-4.17108600
C	-2.39484900	-3.90508700	-3.15167700
C	-2.05370800	-3.56174800	-1.83564800
C	0.19614200	-2.96816400	-2.56709200
C	-0.16293400	-3.38290000	-3.86238400
C	-3.34736800	-1.93247700	0.82378600
C	-3.47799100	-3.26714500	0.43745100
C	-4.06495800	-4.18296400	1.32530400
C	-4.61190000	-3.75565700	2.52964100
C	-4.58588400	-2.39640300	2.83654200
C	-3.95351000	-1.45786600	2.00375400
H	0.59320100	-3.34538100	-4.64089600
H	-5.05016900	-2.03898900	3.75086100
C	-3.17366200	-3.96431600	-0.88579300
C	-4.39957500	-3.89654400	-1.85862400
H	-4.74045300	-2.85626600	-1.92250600
H	-5.24306800	-4.50147300	-1.51172000
H	-4.96617600	-5.93297500	0.41421500
H	-3.65546500	-6.31615400	1.52508000
C	-0.79519800	-3.02678000	-1.56902600
H	-1.70628500	-4.08901200	-5.19195800
H	-5.06810100	-4.46359200	3.21704800
C	-3.84039200	-4.34818200	-3.22604600
H	-4.37625700	-3.90104100	-4.07143100
H	-3.91631100	-5.43780900	-3.34848100
C	-3.98579600	-5.58967600	0.77382300
C	-2.98162600	-5.43648900	-0.38765100
H	-1.95906200	-5.54715100	-0.00904800
H	-3.12324800	-6.17003800	-1.18759500
C	-4.03648000	-0.01131100	2.37961700
C	-3.40289900	0.45762500	3.55548700
C	-4.87362300	0.85249500	1.62944200
C	-2.51874100	-0.35600100	4.33404800
C	-3.63316500	1.81394500	3.99965500

C	-5.07709000	2.21267200	2.07443100
C	-1.92574800	0.12396100	5.47160500
H	-2.28741400	-1.35466500	3.98721400
C	-3.00782100	2.26987400	5.20317100
C	-4.46052300	2.65212000	3.24874900
C	-2.18046400	1.45028100	5.92228600
H	-1.23482800	-0.50694800	6.02294300
H	-3.20643000	3.28763900	5.53205900
H	-4.63000600	3.67269700	3.58648700
H	-1.70540300	1.81025100	6.83100700
C	1.60947000	-2.54896000	-2.31378900
C	2.14848900	-1.43819800	-3.00940700
C	2.44365200	-3.33431800	-1.47803500
C	1.34682800	-0.56025500	-3.81060500
C	3.56213400	-1.15080900	-2.91399000
C	3.84287800	-2.99629500	-1.34601800
C	1.90560600	0.47956100	-4.50876500
H	0.27474600	-0.71402600	-3.84456800
C	4.11009600	-0.07229100	-3.68053800
C	4.36799700	-1.92813300	-2.07821600
C	3.30919700	0.71896300	-4.46127300
H	1.26721700	1.12824800	-5.10163100
H	5.18273300	0.10020000	-3.62755900
H	5.42625300	-1.69218400	-1.99083800
H	3.73894800	1.53039000	-5.04334200
C	-6.38013100	1.29245600	-0.24851300
H	-6.89770800	0.94343100	-1.13825000
C	-5.57181100	0.43341300	0.45054700
H	-5.46294200	-0.59137700	0.11432100
C	-6.55963800	2.63708100	0.18428700
H	-7.20658700	3.30328800	-0.38000900
C	-5.92682500	3.07736200	1.31563800
H	-6.06327400	4.09793300	1.66618500
C	2.80589200	-5.21306000	0.04344300
H	2.41736800	-6.07582400	0.57777300
C	4.17586900	-4.85680000	0.19172600
H	4.81883600	-5.44494100	0.84087200
C	4.67665900	-3.78216900	-0.49075800
H	5.72412200	-3.50465800	-0.39905600
C	1.97447700	-4.48370600	-0.76522800
H	0.93788500	-4.78020000	-0.87017600
C	-1.66643900	3.41789800	-2.06524300
C	-2.25679400	3.07392700	-0.66409300
H	-3.35000200	3.06558500	-0.75738300

H	-1.95932300	2.06020800	-0.38223800
C	-1.86492200	4.01967100	0.44300900
C	-0.13430900	3.61658200	-1.94677700
H	0.03730200	4.48500200	-1.30335300
H	0.29796700	3.82844400	-2.93133200
N	0.58276300	2.47610800	-1.35334300
C	1.80379500	2.57608000	-0.86189600
N	2.39667800	1.55142200	-0.23577000
C	3.73060500	1.52748700	0.28440300
C	4.81782200	1.50708200	-0.58873900
C	3.92466600	1.45579100	1.66839100
C	6.11399900	1.43555400	-0.07283500
C	5.22538100	1.37979600	2.16592300
H	3.06962100	1.44101600	2.33678900
C	6.32376200	1.37230600	1.30258600
H	7.32970300	1.31987600	1.70031200
C	5.44422800	1.25724400	3.65509600
C	7.26785100	1.40840600	-1.04050600
F	6.66252700	1.72513700	4.01256600
F	5.37642000	-0.02629000	4.05991600
F	4.52070400	1.95045600	4.34885100
F	8.46000900	1.37520200	-0.41714700
F	7.25571300	2.49248400	-1.84852600
F	7.20622200	0.32320600	-1.85427900
S	2.61411200	4.14539000	-1.05570500
H	4.64547800	1.52586600	-1.65967200
H	1.84845500	0.70347200	-0.01312700
H	0.11054900	1.55309200	-1.27208500
C	-1.16268200	3.66869300	1.52644200
H	-0.83590800	2.63336000	1.63768800
H	3.69626100	3.81416800	-0.32598800
N	-0.64465500	-0.86731200	1.67878400
S	0.83592800	-0.72950100	2.21700900
O	0.98286100	0.35074000	3.20456100
O	1.87725600	-0.79245000	1.15265400
C	1.08863100	-2.30539400	3.18753300
F	0.19493700	-2.38400400	4.18489400
F	2.31813800	-2.31162000	3.71333400
F	0.94611000	-3.37017200	2.39535900
C	-1.99512800	2.34701900	-3.12756000
C	-2.78519300	1.22302000	-2.85234700
C	-1.51969200	2.50018800	-4.44302100
C	-3.07801200	0.28655900	-3.84767100
H	-3.17420800	1.05154200	-1.85691900

C	-1.81329100	1.57056300	-5.43940700
H	-0.91415600	3.36362800	-4.70769800
C	-2.59511000	0.45179700	-5.14372500
H	-3.68013400	-0.58191800	-3.59570600
H	-1.43370200	1.72326300	-6.44665600
H	-2.82292600	-0.27904000	-5.91493600
C	-2.21624200	4.80515000	-2.55201400
H	-1.92154300	5.57999600	-1.83423400
H	-1.71489200	5.05829200	-3.49752900
C	-3.70517500	4.85881900	-2.75843500
C	-4.52083900	5.73991800	-2.17226300
H	-4.09814200	6.46859300	-1.47721400
H	-4.12308600	4.12967200	-3.45293300
H	-2.21549800	5.05039100	0.36245600
C	-0.80317000	4.58699300	2.65873400
H	-1.21034600	4.21006900	3.60566500
H	0.28555800	4.64670900	2.79316000
H	-1.18317000	5.60217200	2.49670300
C	-6.00350500	5.82686800	-2.39422100
H	-6.55335100	5.69037000	-1.45316900
H	-6.29150400	6.81217600	-2.78550700
H	-6.34914000	5.06656100	-3.10265600

INT-13' -2

0 imaginary frequency

H = -5315.376211

G = -5315.581662

E(M06-2X-DCM) = -5316.271068

E(M06-2X-cyclohexane) = -5316.239360

O	-0.85478100	-2.72442700	-0.26362200
O	-2.66680800	-0.96190100	0.31311400
P	-1.04841100	-1.15472700	0.18414700
O	-0.58692900	-0.21405500	-0.89207900
C	-2.44275900	-3.79226200	-3.99005100
C	-3.24566400	-3.77155800	-2.85413600
C	-2.69340300	-3.49418200	-1.59448600
C	-0.50383400	-3.17973100	-2.62519900
C	-1.07884600	-3.53077800	-3.85905700
C	-3.39963400	-1.74404100	1.20937700
C	-3.76535800	-3.03982700	0.84376800
C	-4.36156900	-3.87747200	1.79972800
C	-4.69017700	-3.39526500	3.06163100
C	-4.42755600	-2.05989100	3.36335100
C	-3.77190400	-1.20868200	2.45798800

H	-0.43423600	-3.57744100	-4.73195800
H	-4.71397700	-1.65720800	4.33036500
C	-3.72874700	-3.75203700	-0.50613900
C	-5.04646700	-3.49988300	-1.31486300
H	-5.24046200	-2.42135900	-1.34284900
H	-5.91575900	-3.98358900	-0.85882000
H	-5.60390100	-5.47130600	1.01055200
H	-4.23338500	-6.04968300	1.95190200
C	-1.35110700	-3.13113300	-1.50041300
H	-2.86394100	-4.01885100	-4.96634000
H	-5.15577500	-4.04183200	3.80121200
C	-4.73574800	-4.01060900	-2.73898400
H	-5.30713400	-3.48357200	-3.51187200
H	-4.97667600	-5.07784900	-2.84347100
C	-4.54861900	-5.27304300	1.24572400
C	-3.68290300	-5.24368600	-0.03159100
H	-2.64696200	-5.50036700	0.21782600
H	-4.02282600	-5.93910900	-0.80546100
C	-3.56155200	0.22172600	2.84634400
C	-2.70633900	0.54372200	3.92813900
C	-4.32085400	1.23741900	2.21223400
C	-1.89152800	-0.43172000	4.58792100
C	-2.62607600	1.91016600	4.39382900
C	-4.20862000	2.60405900	2.67126400
C	-1.08704200	-0.09080200	5.64242800
H	-1.88491200	-1.44724500	4.21325000
C	-1.78406500	2.22032600	5.50791800
C	-3.37155700	2.90109100	3.75037000
C	-1.03987200	1.24934500	6.12065500
H	-0.45776400	-0.84662400	6.10309500
H	-1.74723400	3.25110700	5.85317600
H	-3.30449900	3.92864900	4.10252400
H	-0.39813700	1.49812000	6.96158500
C	0.96788100	-2.91972800	-2.55791800
C	1.52630600	-1.83246900	-3.27465200
C	1.81243200	-3.81667900	-1.85658900
C	0.72763600	-0.86490300	-3.96730400
C	2.96182800	-1.66510400	-3.31684000
C	3.24256800	-3.60967900	-1.86968900
C	1.29973100	0.15956200	-4.67706500
H	-0.35109700	-0.94445500	-3.91082500
C	3.51921900	-0.58352700	-4.07092900
C	3.77959300	-2.55405500	-2.61219200
C	2.71611300	0.30156600	-4.73913400

H	0.66685400	0.87316900	-5.19872100
H	4.60212300	-0.48329500	-4.09914200
H	4.85878100	-2.41905700	-2.63810600
H	3.15244500	1.11402700	-5.31431800
C	-5.97039100	1.97671700	0.56217400
H	-6.66005900	1.74316800	-0.24447200
C	-5.23937100	0.97404000	1.14484400
H	-5.36116300	-0.04605800	0.79926100
C	-5.83937600	3.32429200	1.00513300
H	-6.43278200	4.10602100	0.53771000
C	-4.98194300	3.62331300	2.03083200
H	-4.88379900	4.64453200	2.39259000
C	2.16180900	-5.79428700	-0.46498700
H	1.75641400	-6.64723200	0.07252100
C	3.56601500	-5.56145700	-0.45062700
H	4.21722900	-6.23054400	0.10510300
C	4.08861600	-4.50056500	-1.13841100
H	5.15771900	-4.30545600	-1.13441600
C	1.31781300	-4.95474500	-1.14308700
H	0.25232600	-5.15183400	-1.14278600
C	-1.62191000	3.73197100	-1.69524700
C	-1.28147000	4.43705200	-0.33876200
H	-0.65585700	5.31425900	-0.55324200
H	-2.23139300	4.83896400	0.03845400
C	-0.65378800	3.64400400	0.78283800
C	-0.34599100	3.18703000	-2.38763800
H	0.31465900	4.01914600	-2.63480600
H	-0.62423200	2.68855600	-3.32247100
N	0.41833600	2.22344800	-1.58952700
C	1.70199600	2.29849400	-1.30397700
N	2.29739700	1.32676600	-0.59680300
C	3.62301900	1.33437000	-0.06437400
C	4.48867700	0.29785900	-0.41118400
C	4.02339300	2.31214300	0.85055700
C	5.77062600	0.26027500	0.13860500
C	5.31006000	2.26691900	1.38604300
H	3.32601300	3.08291700	1.15625400
C	6.19106900	1.24328400	1.03302800
H	7.18579200	1.20645600	1.45975900
C	5.76015900	3.36129000	2.32003000
C	6.68764200	-0.86866400	-0.26072700
F	4.73520700	3.84786400	3.05106500
F	6.28287800	4.40432200	1.63153200
F	6.71130500	2.93293300	3.17283300

F	6.81179300	-0.93695900	-1.61122000
F	6.21441300	-2.06491600	0.14402200
F	7.92622600	-0.72384300	0.24955500
S	2.61330000	3.70099500	-1.90461800
H	4.15023800	-0.47617800	-1.08993500
H	1.75771000	0.48052700	-0.35276300
H	-0.06399500	1.35092200	-1.28970500
C	0.30306800	4.13366000	1.58146600
H	0.70034200	5.12820600	1.36064000
H	3.81260900	3.24171000	-1.50025600
N	-0.47194600	-1.04666800	1.68254700
S	1.07727800	-1.05258900	2.02608900
O	1.40902000	-0.10330700	3.09315500
O	1.95645900	-1.06226600	0.82395200
C	1.33786400	-2.73300100	2.79962000
F	2.62233100	-2.87178900	3.14679200
F	1.00981800	-3.70478300	1.94468800
F	0.58031500	-2.85138400	3.89993100
C	-2.26579300	4.80986900	-2.60151800
C	-1.71253100	5.24702700	-3.81430200
C	-3.47524200	5.40587000	-2.19782300
C	-2.32928200	6.23893100	-4.58313000
H	-0.79225400	4.81825400	-4.19524100
C	-4.09318100	6.39417300	-2.96055500
H	-3.95239000	5.08879200	-1.27519200
C	-3.52092500	6.82096400	-4.16048400
H	-1.86956600	6.55056200	-5.51749900
H	-5.02688300	6.83065700	-2.61530900
H	-4.00064200	7.59211100	-4.75692300
C	-2.64256100	2.56434200	-1.48048300
H	-2.18479400	1.76644400	-0.88913000
H	-3.46705700	2.95006600	-0.86780200
C	-3.20230500	1.98616300	-2.75608500
C	-3.07708000	0.71247700	-3.14450000
H	-2.51981100	0.02156000	-2.51349800
H	-3.76704600	2.67396800	-3.38704400
H	-1.08401700	2.66979500	1.01541100
C	0.83898600	3.46763100	2.81901700
H	0.46079800	3.97064200	3.72027100
H	0.55807600	2.41269500	2.88439300
H	1.93335800	3.53023300	2.87745400
C	-3.67600500	0.14265600	-4.39965100
H	-4.20450200	0.90660600	-4.98087500
H	-2.90766100	-0.30698900	-5.04341000

H -4.38781600 -0.66147800 -4.16727100

INT-13' -3

0 imaginary frequency

H = -5315.373773

G = -5315.580042

E(M06-2X-DCM) = -5316.268309

E(M06-2X-cyclohexane) = -5316.239360

O	-0.76371800	-2.59963100	-0.89739100
O	-2.67780200	-1.03988800	-0.10540700
P	-1.04999400	-1.17205700	-0.14432000
O	-0.53070100	-0.01399800	-0.94657300
C	-2.02535700	-2.85635000	-4.88255400
C	-2.90474600	-3.12177000	-3.83791700
C	-2.45616000	-3.11035700	-2.50912400
C	-0.22387100	-2.47286200	-3.26666500
C	-0.69271200	-2.56705200	-4.58912800
C	-3.44452300	-2.01604000	0.53670200
C	-3.72069300	-3.21503700	-0.12220500
C	-4.34810700	-4.25293600	0.58571500
C	-4.79467000	-4.05874300	1.88797300
C	-4.62059500	-2.80980300	2.48252300
C	-3.93823100	-1.76806200	1.83280100
H	0.00918700	-2.38319600	-5.39727200
H	-4.99978800	-2.62917000	3.48405900
C	-3.55192400	-3.62648600	-1.58410600
C	-4.81947200	-3.24859000	-2.42435500
H	-5.06106000	-2.19546200	-2.23991600
H	-5.69519900	-3.84540900	-2.15115100
H	-5.45138600	-5.68267000	-0.61605600
H	-4.12844000	-6.40325200	0.29461500
C	-1.14607100	-2.72710200	-2.23250800
H	-2.36434700	-2.87717100	-5.91532800
H	-5.28376200	-4.86128000	2.43434600
C	-4.38465400	-3.43222900	-3.89496500
H	-4.92648100	-2.77215100	-4.58200400
H	-4.56316800	-4.46041700	-4.24005100
C	-4.42691400	-5.50579700	-0.25921000
C	-3.47152100	-5.18200500	-1.42720100
H	-2.44589500	-5.45424300	-1.15298000
H	-3.72092900	-5.70863000	-2.35374900
C	-3.82651300	-0.44376600	2.52369200
C	-3.04389100	-0.31677200	3.69675400
C	-4.60699300	0.64834600	2.06734200

C	-2.22529800	-1.37852600	4.19925700
C	-3.04557800	0.93178800	4.42623200
C	-4.58801900	1.89518700	2.79965500
C	-1.48386600	-1.22646200	5.34049400
H	-2.16577300	-2.30226100	3.63865800
C	-2.26479300	1.04495700	5.61950700
C	-3.81056900	2.00222700	3.95628600
C	-1.50894500	-0.00338900	6.06891800
H	-0.84888800	-2.03949800	5.67955400
H	-2.28568600	1.98862400	6.15990900
H	-3.80871800	2.93924800	4.50986400
H	-0.91496500	0.09589100	6.97347400
C	1.21375400	-2.13391600	-3.02751100
C	1.72413900	-0.88579300	-3.46517900
C	2.08491100	-3.09083000	-2.44931100
C	0.89483800	0.14638600	-4.01524000
C	3.13912500	-0.61117700	-3.35233700
C	3.48930900	-2.78238200	-2.30096100
C	1.42329000	1.33051700	-4.46219200
H	-0.17441800	-0.01967600	-4.06804800
C	3.65429000	0.63007300	-3.84762600
C	3.98065400	-1.55904000	-2.76433200
C	2.82531400	1.57527500	-4.39130100
H	0.76774800	2.08942100	-4.88218000
H	4.72714700	0.79900400	-3.78601200
H	5.04071300	-1.33613700	-2.66182400
H	3.23077200	2.50930100	-4.77162600
C	-6.21905400	1.63840600	0.51475400
H	-6.85893900	1.54578400	-0.35864400
C	-5.45924000	0.57111000	0.91846300
H	-5.50635400	-0.35926300	0.36424100
C	-6.18439400	2.86881000	1.23164500
H	-6.80074400	3.70198700	0.90371400
C	-5.38951100	2.98828700	2.34115200
H	-5.36645000	3.91524300	2.91022000
C	2.51064400	-5.28209900	-1.45485200
H	2.14510200	-6.25314800	-1.13200500
C	3.88734400	-4.96162400	-1.28724200
H	4.55798400	-5.68613700	-0.83343600
C	4.35942900	-3.74743500	-1.70478300
H	5.41048600	-3.49178300	-1.59383400
C	1.64444400	-4.38287900	-2.01875900
H	0.60228800	-4.65115800	-2.14517100
C	-1.63825300	3.93755500	-0.65212300

C	-1.50177100	4.38758700	0.84378300
H	-1.03351800	5.38139700	0.86810900
H	-2.52433400	4.53173500	1.21761900
C	-0.78066600	3.47561300	1.80303000
C	-0.25690300	3.61909200	-1.28029400
H	0.38707800	4.49699900	-1.24728700
H	-0.39945900	3.36063400	-2.33524400
N	0.47281300	2.49278800	-0.68185500
C	1.72751300	2.48024700	-0.27214800
N	2.35055900	1.32768700	-0.00956200
C	3.71271800	1.20146400	0.42006500
C	3.99848300	0.77688500	1.72031300
C	4.73424800	1.43679300	-0.49553400
C	5.33133800	0.61583400	2.09717800
C	6.06374900	1.26144000	-0.10519700
H	4.48812700	1.72417400	-1.51225600
C	6.36820300	0.85557800	1.19103200
H	7.39941600	0.72393800	1.49481300
C	7.14202300	1.49381200	-1.12916400
C	5.65476300	0.12325800	3.48686400
F	8.37492600	1.26571300	-0.64010200
F	7.11417800	2.75993300	-1.60052400
F	6.97604500	0.68064600	-2.20596900
F	4.76769100	0.57840500	4.39311700
F	6.88527200	0.52735500	3.87879900
F	5.64142000	-1.22394500	3.54983500
S	2.66851200	3.97748400	-0.01269100
H	3.19120500	0.56359800	2.41336500
H	1.84148100	0.43377300	-0.08713000
H	0.02272500	1.55366200	-0.76477400
C	0.12931200	3.89182200	2.69352100
H	0.38924100	4.95461700	2.71776900
H	1.63121000	4.62421500	0.56103500
N	-0.59270600	-1.37734000	1.38856400
S	0.92397100	-1.49363400	1.82894900
O	1.20773600	-0.72921800	3.05384900
O	1.89478300	-1.34064000	0.71164000
C	1.09096400	-3.28265700	2.34165600
F	2.34281800	-3.51395700	2.74919800
F	0.80713300	-4.09146300	1.31820200
F	0.25238800	-3.55331100	3.35304000
C	-2.27358300	5.12271400	-1.41684900
C	-1.64259000	5.80161200	-2.46997400
C	-3.54797400	5.58033500	-1.03388200

C	-2.25117200	6.88580100	-3.10949800
H	-0.66358500	5.49778500	-2.82341200
C	-4.15761100	6.66124700	-1.66700000
H	-4.08353100	5.08336400	-0.23052900
C	-3.51097700	7.32405900	-2.71170600
H	-1.73052200	7.38392500	-3.92334900
H	-5.14313900	6.98494700	-1.34204200
H	-3.98449200	8.16694600	-3.20761200
C	-2.58275200	2.69121400	-0.75149400
H	-2.19207000	1.89483300	-0.10995900
H	-3.55203400	2.96784100	-0.32749700
C	-2.77522100	2.13445800	-2.14034900
C	-3.83818600	2.36643700	-2.91629700
H	-4.63384500	3.01296300	-2.54292600
H	-1.99473300	1.46700200	-2.50524900
H	-1.07196600	2.42569300	1.81254200
C	0.81138100	3.02039100	3.71075400
H	0.54273200	1.96579000	3.59527800
H	1.90455500	3.10387500	3.63682400
H	0.54664500	3.32794300	4.73163100
C	-4.04249400	1.79576600	-4.29071200
H	-4.12826000	2.59050300	-5.04479800
H	-3.21544900	1.13843400	-4.58071600
H	-4.97208700	1.21246700	-4.34588700

INT-13-1

0 imaginary frequency

H = -5315.395953

G = -5315.599031

E(M06-2X-DCM) = -5316.279016

E(M06-2X-cyclohexane) = -5316.254695

C	-3.25225800	3.78500700	-0.43221500
C	-4.20415800	3.30318400	0.70427300
H	-3.83802100	2.34215400	1.08415600
H	-4.13527800	4.02494400	1.52808100
C	-5.65568300	3.16589900	0.32483200
C	-3.24943800	2.74968800	-1.59158800
H	-2.68752000	3.14607200	-2.44820000
H	-4.27288100	2.57664900	-1.92548600
N	-2.69985200	1.45707800	-1.20892600
C	-3.16788900	0.25754200	-1.64197500
N	-2.36603800	-0.78914500	-1.22711400
C	-2.57094500	-2.17124600	-1.32596300
C	-3.83965600	-2.77455600	-1.30834400

C	-1.43364500	-2.99157900	-1.36786600
C	-3.94862100	-4.16194100	-1.36249700
C	-1.56413000	-4.37927700	-1.41349400
H	-0.44616700	-2.54200300	-1.35931600
C	-2.82043400	-4.98113400	-1.42445100
H	-2.91976300	-6.05842300	-1.47847200
C	-0.33298300	-5.23679800	-1.36662700
C	-5.30724100	-4.80171200	-1.25082800
F	0.71606300	-4.66452100	-2.00463500
F	-0.52730100	-6.45177700	-1.91683900
F	0.07515400	-5.45343100	-0.08277700
F	-5.37620300	-5.95856200	-1.94646000
F	-6.29378000	-3.99875600	-1.69087400
F	-5.59913700	-5.11257700	0.04166700
S	-4.54395300	0.07990300	-2.60520900
H	-4.72650300	-2.16037400	-1.25921500
C	-6.31166900	2.00698800	0.21609300
H	-1.44069500	-0.52133100	-0.88939500
H	-1.77722900	1.46956700	-0.78002200
H	1.04587700	2.04412300	1.55784300
O	1.08926400	-1.31052000	1.01864200
O	2.83234800	-0.00068600	-0.36774600
P	1.38779200	0.11529200	0.33235400
O	0.20768500	0.50307200	-0.47801000
C	3.52953700	-2.58719100	4.16693000
C	3.97290700	-2.69123800	2.85353400
C	3.11782100	-2.38501800	1.78242000
C	1.37439200	-1.74533300	3.37915200
C	2.22360800	-2.16142800	4.41631200
C	3.08843800	-1.00024000	-1.33409600
C	3.43825900	-2.27894100	-0.90717100
C	3.59903600	-3.28234900	-1.87891000
C	3.49199400	-2.99142100	-3.23411500
C	3.21456500	-1.68441700	-3.63176700
C	2.99312000	-0.66123800	-2.69686100
H	1.85361400	-2.11468100	5.43617400
H	3.14434100	-1.43962500	-4.68740500
C	3.76309000	-2.84209300	0.47637100
C	5.27247700	-2.67162300	0.84923700
H	5.93063400	-3.26305400	0.20512500
H	5.54703700	-1.61628700	0.74011800
H	3.27116900	-5.42300200	-1.68987800
H	4.91553000	-4.90502900	-1.31327700
C	1.87800400	-1.82733400	2.06737700

H	4. 18734200	-2. 83664400	4. 99545700
H	3. 61831400	-3. 77312700	-3. 97842700
C	5. 34387100	-3. 07764600	2. 33986500
H	5. 53210600	-4. 15367300	2. 45585900
H	6. 14429200	-2. 55742500	2. 87737400
C	3. 85715500	-4. 62155300	-1. 22925300
C	3. 45226100	-4. 36091400	0. 23423900
H	3. 96784000	-5. 00696700	0. 95038500
H	2. 37718900	-4. 52867700	0. 34719200
C	2. 69916400	0. 72623500	-3. 18163000
C	3. 73097200	1. 69558200	-3. 18023000
C	1. 42563300	1. 03755200	-3. 71350300
C	5. 06328700	1. 41038500	-2. 74106200
C	3. 45820200	3. 02754700	-3. 67028100
C	1. 17005700	2. 37096600	-4. 21201000
C	6. 04241800	2. 36961900	-2. 76042200
H	5. 29688700	0. 41025200	-2. 39273500
C	4. 50402600	4. 00267000	-3. 66046900
C	2. 18541800	3. 32966000	-4. 16338400
C	5. 76083200	3. 68819000	-3. 21804800
H	7. 04642800	2. 12313500	-2. 42547000
H	4. 27869000	5. 00191500	-4. 02587700
H	1. 98701800	4. 33152000	-4. 53968900
H	6. 54860000	4. 43650000	-3. 22265500
C	-0. 01568600	-1. 27072700	3. 66956300
C	-1. 12051000	-2. 05971800	3. 25997000
C	-0. 22696300	-0. 06558200	4. 38435700
C	-0. 97525100	-3. 31526100	2. 58779500
C	-2. 46457100	-1. 60672800	3. 53995900
C	-1. 57810700	0. 37107400	4. 66191000
C	-2. 06608200	-4. 04881700	2. 20089100
H	0. 01950300	-3. 69483100	2. 38440200
C	-3. 57547700	-2. 39688200	3. 10735100
C	-2. 65538500	-0. 40523300	4. 22752700
C	-3. 38793200	-3. 58259700	2. 45013500
H	-1. 91786200	-4. 99221600	1. 68547700
H	-4. 57788000	-2. 02868700	3. 31259600
H	-3. 66927900	-0. 06835100	4. 43421500
H	-4. 23642500	-4. 16374700	2. 10210200
C	-0. 85676100	0. 41448300	-4. 32939500
H	-1. 65277300	-0. 32266600	-4. 37396600
C	0. 36011600	0. 08342100	-3. 79361100
H	0. 53005000	-0. 92217900	-3. 42529400
C	-1. 10313000	1. 73055900	-4. 81661200

H	-2.07737200	1.97033600	-5.23254100
C	-0.11712300	2.67823400	-4.75588700
H	-0.28901700	3.68430200	-5.13216100
C	0.60275300	1.93623100	5.51960700
H	1.43860500	2.55045800	5.84120800
C	-0.72964000	2.35810900	5.79333800
H	-0.90150700	3.28367000	6.33609900
C	-1.78589300	1.59475600	5.37298100
H	-2.80907100	1.90260900	5.57588100
C	0.84366800	0.76920000	4.84132000
H	1.86535700	0.46792800	4.64224000
N	1.75633400	1.30961300	1.47656200
S	3.21071000	1.77729300	2.19395800
C	4.23977400	2.54114900	0.79446800
O	3.94915300	0.60673700	2.64004500
O	2.86722200	2.88641800	3.07553400
F	3.44601100	2.98372600	-0.17824200
F	4.91527200	3.56375400	1.31720400
F	5.09226900	1.63880800	0.32651700
H	-6.20212200	4.09459100	0.15656400
H	-5.76807800	1.07667700	0.38424500
C	-1.81677500	4.01356200	0.08842700
C	-1.45464500	3.85863400	1.43538100
C	-0.80813900	4.42672400	-0.80370100
C	-0.15834200	4.14548600	1.88055300
H	-2.18186800	3.52254700	2.16492900
C	0.48598600	4.70550500	-0.37054600
H	-1.03267900	4.53380700	-1.86096300
C	0.81568800	4.58286700	0.98125600
H	0.08274100	4.03377100	2.93460600
H	1.23809200	5.01582700	-1.09068100
H	1.81682900	4.81515500	1.33110900
C	-3.78607400	5.12144100	-1.04959800
H	-3.10568400	5.41492100	-1.86156800
H	-4.75644200	4.92710200	-1.52129700
C	-3.91409800	6.26434200	-0.07905700
H	-3.01208200	6.53151100	0.47370700
C	-5.02959900	6.97079900	0.12854400
H	-5.93106600	6.70748600	-0.42887100
C	-7.76052000	1.86166100	-0.14758200
H	-7.87102100	1.26856600	-1.06478500
H	-8.31961200	1.33498200	0.63808200
H	-8.23728400	2.83486900	-0.30895700
C	-5.15583900	8.13177300	1.07355800

H	-5.45075900	9.04743300	0.54293000
H	-5.92946200	7.94706200	1.83125900
H	-4.21270300	8.33128900	1.59360300

INT-13-2

0 imaginary frequency

H = -5315.394607

G = -5315.598647

E(M06-2X-DCM) = -5316.278474

E(M06-2X-cyclohexane) = -5316.253691

C	-1.72564700	4.71223000	-0.35513100
C	-2.79182700	4.57991100	0.77521900
H	-2.80837200	3.53869200	1.11771800
H	-2.46241800	5.18792100	1.62742100
C	-4.19116400	5.00031300	0.40527500
C	-2.09423400	3.76143100	-1.52908700
H	-1.42785900	3.94309500	-2.38307500
H	-3.11201800	3.97006800	-1.86016500
N	-2.04252700	2.35228400	-1.16716400
C	-2.91692900	1.40726900	-1.60073300
N	-2.54125000	0.13734700	-1.20561900
C	-3.22859600	-1.07825900	-1.31577700
C	-4.62887800	-1.18799700	-1.28721700
C	-2.46043600	-2.25037000	-1.38184300
C	-5.22757300	-2.44367200	-1.35513200
C	-3.07922200	-3.49869800	-1.44091000
H	-1.37742900	-2.18372800	-1.38177000
C	-4.46780500	-3.61109300	-1.44164000
H	-4.94654800	-4.58062200	-1.50629400
C	-2.23631200	-4.74061600	-1.41959600
C	-6.72415100	-2.55683200	-1.23220800
F	-2.85558000	-5.79606200	-1.98460800
F	-1.92612400	-5.11080500	-0.14343200
F	-1.05530300	-4.57082800	-2.06098000
F	-7.20842700	-3.60189900	-1.93945700
F	-7.36187300	-1.44762800	-1.65016100
F	-7.09687400	-2.76204300	0.06059700
S	-4.27688600	1.74889400	-2.54267500
H	-5.23663600	-0.29804300	-1.21893300
C	-5.23227100	4.17115000	0.28748600
H	-1.57887400	0.05059500	-0.87624400
H	-1.17291600	2.02669300	-0.75103000
H	1.67374500	1.51709200	1.56945300
O	0.51298200	-1.62662200	0.99630100

O	2. 59928800	-1. 00427800	-0. 39585200
P	1. 29554900	-0. 39142500	0. 32178600
O	0. 32642600	0. 40145200	-0. 47319300
C	2. 36081400	-3. 74655100	4. 09321900
C	2. 72709500	-3. 97903600	2. 77257000
C	2. 02969500	-3. 36867400	1. 71739700
C	0. 64341700	-2. 17589900	3. 34652700
C	1. 29574600	-2. 88650100	4. 36614300
C	2. 47507600	-2. 01212100	-1. 37940200
C	2. 34678700	-3. 33849400	-0. 97456100
C	2. 13193200	-4. 31633000	-1. 96170500
C	2. 12800800	-3. 98327600	-3. 31140200
C	2. 33436700	-2. 65692900	-3. 68760800
C	2. 49929100	-1. 63825800	-2. 73617400
H	0. 97505900	-2. 72849500	5. 39150500
H	2. 35010400	-2. 38515600	-4. 73884900
C	2. 45837300	-4. 00404400	0. 39691800
C	3. 93174900	-4. 39119000	0. 75161000
H	4. 32965700	-5. 16759300	0. 09078100
H	4. 56498300	-3. 50219700	0. 65290200
H	1. 06074200	-6. 20074200	-1. 79759100
H	2. 78402800	-6. 31213300	-1. 43475500
C	1. 07366300	-2. 40944000	2. 02685800
H	2. 89234500	-4. 22942700	4. 90912400
H	1. 96183400	-4. 74557800	-4. 06791800
C	3. 86460200	-4. 82171500	2. 23541400
H	3. 65565700	-5. 89564900	2. 33427400
H	4. 80239200	-4. 63214700	2. 76912400
C	1. 89796900	-5. 67010200	-1. 33352600
C	1. 62333400	-5. 30715500	0. 13844600
H	1. 87921400	-6. 10700600	0. 83904400
H	0. 56015000	-5. 08191000	0. 26320400
C	2. 71808800	-0. 22963700	-3. 19921600
C	4. 02796400	0. 30746800	-3. 19505700
C	1. 63742400	0. 52385100	-3. 71523500
C	5. 17247000	-0. 44102000	-2. 77178300
C	4. 24678500	1. 65614400	-3. 66609200
C	1. 87296800	1. 86756800	-4. 19557200
C	6. 42942900	0. 10575300	-2. 78803700
H	5. 03500600	-1. 46366300	-2. 43797600
C	5. 57183300	2. 19354700	-3. 65352600
C	3. 16392100	2. 39976400	-4. 14442100
C	6. 63531500	1. 44466500	-3. 22651700
H	7. 28062500	-0. 48783400	-2. 46538000

H	5.71656800	3.21274700	-4.00434300
H	3.33486800	3.41176300	-4.50679800
H	7.63829900	1.86250300	-3.22890100
C	-0.48182400	-1.24069300	3.66442800
C	-1.79939600	-1.57282400	3.25874000
C	-0.24138000	-0.05577400	4.40357200
C	-2.11939000	-2.78209800	2.56260600
C	-2.88975100	-0.67546200	3.56856200
C	-1.34437200	0.82847500	4.71154500
C	-3.40392300	-3.06811500	2.18070400
H	-1.32848500	-3.48803600	2.33657600
C	-4.21369900	-1.00605600	3.14019300
C	-2.63187500	0.49875300	4.28091000
C	-4.46899600	-2.16549600	2.45938800
H	-3.60780500	-3.99064800	1.64689400
H	-5.01597600	-0.30829600	3.36827500
H	-3.45630900	1.17088300	4.51064500
H	-5.47238200	-2.39696400	2.11524400
C	-0.71970700	0.76631200	-4.31704900
H	-1.72680900	0.36293600	-4.36249600
C	0.30085900	0.01480100	-3.79628100
H	0.10167000	-0.99000000	-3.44071100
C	-0.48153300	2.09010300	-4.78713600
H	-1.30747800	2.66790700	-5.19160600
C	0.77827100	2.62200100	-4.72427500
H	0.97562300	3.62830900	-5.08717600
C	1.25976100	1.49119800	5.56026100
H	2.26299300	1.75906000	5.87824400
C	0.16891000	2.35470200	5.86429300
H	0.34447100	3.26803000	6.42624700
C	-1.09427400	2.02889900	5.44812700
H	-1.93778500	2.67734600	5.67365600
C	1.06114200	0.33087400	4.85725600
H	1.90577400	-0.31063300	4.63539400
N	2.07241100	0.57714200	1.47499800
S	3.60000100	0.48106000	2.18640000
C	4.83092200	0.84542500	0.78930600
O	3.86998500	-0.88327600	2.61111400
O	3.68091700	1.62609500	3.08496000
F	5.83357700	1.54277200	1.32192900
F	5.29627500	-0.29559800	0.29753300
F	4.24833000	1.56444900	-0.16752600
H	-4.35765100	6.06721500	0.24613300
H	-5.07351000	3.10338400	0.44119600

C	-0.30553800	4.40345300	0.16193100
C	-0.02262600	4.10800200	1.50357200
C	0.78310900	4.43773300	-0.73050700
C	1.29019500	3.90307700	1.94526000
H	-0.82098000	4.04384000	2.23336600
C	2.09132800	4.22714300	-0.30154200
H	0.61132200	4.63225500	-1.78522300
C	2.35599400	3.97521700	1.04667000
H	1.47545300	3.69604700	2.99623100
H	2.90418700	4.25605800	-1.02205200
H	3.37401500	3.82807500	1.39399600
C	-1.74359000	6.16104300	-0.95450600
H	-0.99725100	6.22229100	-1.75460500
H	-2.72082800	6.30466200	-1.43577900
C	-1.50266500	7.27275500	0.03086700
H	-2.27406500	7.43517600	0.78543500
C	-0.43149300	8.07117900	0.03556800
H	0.34292800	7.91422500	-0.71758600
C	-6.63125700	4.58049500	-0.06926200
H	-6.71202100	5.66313600	-0.21676500
H	-6.95525600	4.08273500	-0.99251500
H	-7.34501100	4.28913400	0.71353000
C	-0.18912700	9.19077900	1.00663100
H	-1.00909600	9.28407400	1.72696100
H	0.74095700	9.03336300	1.56955300
H	-0.08207300	10.15333900	0.48797600

INT-13-3

0 imaginary frequency

H = -5315.392945

G = -5315.597795

E(M06-2X-DCM) = -5316.276035

E(M06-2X-cyclohexane) = -5316.251170

C	4.34856800	-2.24128200	0.37237900
C	5.39142500	-3.05512500	1.21345100
H	4.92459500	-3.34172300	2.16504900
H	5.60277400	-3.98920100	0.68125100
C	6.68825000	-2.35119500	1.52337900
C	3.97916300	-0.96125800	1.17699700
H	4.86699000	-0.35319900	1.35031100
H	3.57537000	-1.25068800	2.15790900
N	3.02152700	-0.10238400	0.50086800
C	3.14226100	1.24453300	0.36814400
N	2.00727700	1.80751100	-0.18001800

C	1. 72978700	3. 15927800	-0. 43827700
C	2. 66986400	4. 04664900	-0. 98668100
C	0. 42764100	3. 61352000	-0. 19104500
C	2. 30368100	5. 36481500	-1. 25271600
C	0. 07717600	4. 93545800	-0. 47178500
H	-0. 29726500	2. 93988900	0. 25457100
C	1. 01008900	5. 82518100	-0. 99937800
H	0. 73808100	6. 85153300	-1. 21173600
C	-1. 33488100	5. 38167800	-0. 21990000
C	3. 33665600	6. 32493200	-1. 78379200
F	-1. 81621700	4. 89421700	0. 95560700
F	-2. 18340600	4. 94168100	-1. 18520300
F	-1. 45475300	6. 72265500	-0. 17375300
F	3. 99135400	6. 95705600	-0. 78437400
F	2. 77408000	7. 28653700	-2. 55267100
F	4. 26804300	5. 69978500	-2. 53489700
S	4. 50896800	2. 11975100	0. 83321200
H	3. 67333200	3. 70476100	-1. 19586600
C	7. 89869900	-2. 79262200	1. 16880500
H	1. 20177400	1. 18600100	-0. 25705800
H	2. 13710000	-0. 52423800	0. 22745000
H	-0. 52977700	-2. 64832800	1. 02768300
O	-1. 64857500	0. 56888600	1. 19506200
O	-2. 58760800	-0. 77877200	-0. 79327200
P	-1. 32041800	-0. 64545700	0. 18899000
O	0. 03383900	-0. 43330100	-0. 37744200
C	-4. 83783500	0. 17339600	3. 86885600
C	-5. 08011300	0. 48942900	2. 53671800
C	-4. 01622000	0. 74848900	1. 65748000
C	-2. 43041600	0. 25285000	3. 45749800
C	-3. 52092200	0. 10389500	4. 32809800
C	-3. 01349600	0. 32247100	-1. 57065400
C	-3. 85003200	1. 27491900	-0. 99482200
C	-4. 18801100	2. 40790300	-1. 75618100
C	-3. 76319600	2. 53917100	-3. 07340100
C	-2. 98630300	1. 53186000	-3. 64414900
C	-2. 58205800	0. 40804700	-2. 90735500
H	-3. 32162200	-0. 10083200	5. 37574100
H	-2. 66095000	1. 61406200	-4. 67694600
C	-4. 56493300	1. 32661200	0. 35561000
C	-5. 96312500	0. 62613600	0. 32069600
H	-6. 67532400	1. 14694000	-0. 32679900
H	-5. 83831800	-0. 39352900	-0. 06112900
H	-4. 67100000	4. 41583100	-1. 07630500

H	-6.06334900	3.33865100	-1.20620800
C	-2.72186800	0.52810300	2.10875900
H	-5.66185500	-0.01458700	4.55226300
H	-4.02732000	3.41936800	-3.65332000
C	-6.40193100	0.57800100	1.80325000
H	-6.96316500	1.47893200	2.08634700
H	-7.04961600	-0.27850300	2.02030400
C	-4.99943700	3.38212800	-0.93455600
C	-4.75905300	2.87703900	0.50084600
H	-5.56593100	3.13018000	1.19437900
H	-3.83460700	3.31840500	0.88693800
C	-1.74636000	-0.64763800	-3.56572000
C	-2.36060500	-1.84425200	-4.00692800
C	-0.37138100	-0.41781700	-3.80725200
C	-3.76308000	-2.09435200	-3.86493100
C	-1.56194600	-2.85757800	-4.65814500
C	0.41456300	-1.43678000	-4.46715100
C	-4.32870300	-3.26106300	-4.30968800
H	-4.38538900	-1.33749200	-3.40018300
C	-2.18903800	-4.06563800	-5.09655900
C	-0.19770200	-2.62945900	-4.86253500
C	-3.53257300	-4.26676500	-4.92807200
H	-5.39710500	-3.42194100	-4.19306900
H	-1.57139800	-4.82010300	-5.57817500
H	0.39859500	-3.39185000	-5.36031400
H	-3.99796300	-5.18658000	-5.27138700
C	-1.02118300	0.16140300	3.95311900
C	-0.20830700	1.32369100	3.94826900
C	-0.50937600	-1.06481900	4.44485500
C	-0.68110100	2.60409500	3.51564700
C	1.15931300	1.24034500	4.40797900
C	0.85742600	-1.12844500	4.91539200
C	0.13773100	3.70362300	3.50820500
H	-1.71146800	2.70547400	3.19407800
C	1.98295200	2.40880600	4.37625800
C	1.65322700	0.01949100	4.87638500
C	1.49200800	3.60729100	3.93501200
H	-0.25090000	4.65629900	3.16115200
H	3.01567200	2.31993700	4.70258800
H	2.68307300	-0.03605000	5.22333400
H	2.13141800	4.48444300	3.90482300
C	1.62476500	0.98705500	-3.69057200
H	2.10192500	1.91725800	-3.39655300
C	0.29342200	0.79360800	-3.43081700

H	-0.27540600	1.57057400	-2.93218600
C	2.39538400	-0.02207200	-4.33632700
H	3.45011900	0.14968600	-4.53186100
C	1.80423300	-1.19902500	-4.70994600
H	2.37965200	-1.97494600	-5.20955000
C	-0.74657300	-3.44545700	4.95487200
H	-1.35418800	-4.34558800	4.95809700
C	0.59584600	-3.49885200	5.42712600
H	0.99791500	-4.43532600	5.80422200
C	1.37151200	-2.37075600	5.40437500
H	2.39810800	-2.39526900	5.76289600
C	-1.27824800	-2.27303300	4.48329200
H	-2.30158100	-2.25533500	4.12697100
N	-1.42562000	-2.15773000	0.94763100
S	-2.72089700	-3.20988000	1.20704500
C	-3.22960700	-3.82293000	-0.51475500
O	-3.86599300	-2.47673600	1.72257200
O	-2.14524000	-4.36840900	1.87837200
F	-4.24269500	-3.09624200	-0.96896700
F	-2.19714600	-3.75982600	-1.35353200
F	-3.61647700	-5.09048800	-0.38000200
H	6.62622700	-1.43674800	2.11515600
H	7.97087300	-3.70941900	0.58153100
C	3.06904500	-3.08728000	0.18957300
C	2.45977100	-3.69645900	1.30312700
C	2.42725600	-3.24135200	-1.05060800
C	1.29830600	-4.46032100	1.17890700
H	2.88722200	-3.57656900	2.29373400
C	1.26539100	-4.00568900	-1.18425800
H	2.82292200	-2.75707500	-1.93540500
C	0.70222100	-4.63366100	-0.07421800
H	0.85822600	-4.91851400	2.06030300
H	0.79766700	-4.09720400	-2.16065700
H	-0.19364000	-5.23877100	-0.17439700
C	4.99690000	-1.80710000	-0.97331800
H	4.25785200	-1.22947900	-1.54508400
H	5.80288400	-1.10289200	-0.74034500
C	5.55491500	-2.91873600	-1.82726000
H	4.89824400	-3.76379900	-2.03724300
C	6.78167700	-2.92444200	-2.35783600
H	7.44895000	-2.08675100	-2.14765500
C	9.19818000	-2.12417600	1.51592100
H	9.03856300	-1.20899900	2.09601000
H	9.84546600	-2.79052200	2.10269200

H	9.76249100	-1.85776800	0.61178200
C	7.33551000	-4.00420200	-3.24384800
H	7.61693800	-3.60755400	-4.22919700
H	8.24572200	-4.44606300	-2.81544700
H	6.60957900	-4.80999000	-3.39910200

INT-13-4

0 imaginary frequency

H = -5315.390930

G = -5315.597172

E(M06-2X-DCM) = -5316.272599

E(M06-2X-cyclohexane) = -5316.246306

C	-3.26419200	3.92452900	1.13812100
C	-3.79372600	3.02440200	2.30853500
H	-3.17754300	2.11907600	2.35298900
H	-3.62137400	3.55908200	3.25092100
C	-5.24670500	2.63311500	2.24133700
C	-3.50776700	3.21020000	-0.21326400
H	-3.15010200	3.83078800	-1.04320800
H	-4.58124800	3.08138900	-0.35554800
N	-2.91957100	1.87583200	-0.29000800
C	-3.47393000	0.82361700	-0.94092000
N	-2.65715500	-0.29477400	-0.91337800
C	-2.95515200	-1.61506600	-1.27006300
C	-4.23010800	-2.18608400	-1.11615900
C	-1.90367200	-2.42309600	-1.72666700
C	-4.43627600	-3.52353100	-1.44302400
C	-2.12977400	-3.76293400	-2.04334700
H	-0.91002000	-2.00089000	-1.83326200
C	-3.39770200	-4.32607600	-1.91858600
H	-3.57448900	-5.36131200	-2.18428800
C	-0.97539500	-4.63060900	-2.45139000
C	-5.78048200	-4.15172900	-1.18765700
F	-0.03112800	-3.94198500	-3.13569100
F	-1.35521100	-5.67022500	-3.22052400
F	-0.34356300	-5.16539400	-1.36502300
F	-6.78189600	-3.25270800	-1.19577900
F	-5.81277200	-4.76605900	0.02741100
F	-6.07238800	-5.10286900	-2.10233900
S	-4.96657100	0.88762900	-1.72711100
H	-5.04818600	-1.58332000	-0.75013500
C	-5.69327000	1.38394100	2.08251600
H	-1.67367000	-0.12256100	-0.69894600
H	-1.97077200	1.76754000	0.05631300

H	1. 62267400	0. 44599700	2. 47834800
O	1. 15686500	-1. 62069500	0. 53283200
O	2. 70828600	0. 02469500	-0. 75002700
P	1. 40715400	-0. 06257700	0. 18585000
O	0. 13583300	0. 51806400	-0. 30515300
C	4. 13854500	-3. 71387200	2. 59038900
C	4. 28296100	-3. 45305600	1. 23179800
C	3. 24431700	-2. 85288800	0. 49883800
C	1. 92720900	-2. 67664100	2. 55711400
C	2. 94910800	-3. 36306000	3. 23143400
C	2. 70618600	-0. 62051400	-2. 00618100
C	3. 02192000	-1. 97583800	-2. 05369900
C	2. 91202600	-2. 64414300	-3. 28418100
C	2. 58250800	-1. 95030900	-4. 44381200
C	2. 35810900	-0. 57560000	-4. 37719200
C	2. 40020900	0. 12227500	-3. 15899800
H	2. 81025200	-3. 59406700	4. 28336800
H	2. 12331500	-0. 01888400	-5. 27939500
C	3. 56750600	-2. 92948100	-0. 99273900
C	5. 13108100	-2. 90680900	-0. 93193600
H	5. 58856600	-3. 30784000	-1. 84123400
H	5. 46678100	-1. 87108500	-0. 81230900
H	2. 43924500	-4. 73604400	-3. 64536600
H	4. 16461800	-4. 39798300	-3. 50096900
C	2. 12706500	-2. 39763800	1. 19167700
H	4. 93779600	-4. 19235900	3. 15051200
H	2. 50067100	-2. 47023200	-5. 39464500
C	5. 47690000	-3. 71582800	0. 33860200
H	5. 58356500	-4. 78650700	0. 11792000
H	6. 41800400	-3. 39530700	0. 79960900
C	3. 17361600	-4. 12302700	-3. 11383900
C	3. 09062300	-4. 30159600	-1. 58402400
H	3. 68507500	-5. 14110800	-1. 21182400
H	2. 05029400	-4. 47498900	-1. 29487500
C	2. 15848200	1. 59858500	-3. 13645200
C	3. 24792400	2. 47829400	-2. 92641900
C	0. 86222500	2. 10664900	-3. 39107700
C	4. 58806100	2. 02266600	-2. 71082700
C	3. 02360800	3. 90535800	-2. 95453400
C	0. 65503300	3. 53721000	-3. 42366200
C	5. 61932500	2. 90412000	-2. 51859000
H	4. 78680500	0. 95658700	-2. 70907600
C	4. 12639700	4. 79072000	-2. 74329900
C	1. 73706600	4. 39369400	-3. 20134100

C	5.38897100	4.30893300	-2.52875000
H	6.62706800	2.52945700	-2.35939300
H	3.93637200	5.86127100	-2.76156500
H	1.57459000	5.46942000	-3.22645300
H	6.21891800	4.99219600	-2.37107000
C	0.67260300	-2.27439900	3.26864000
C	-0.55873400	-2.88644800	2.92087900
C	0.72036900	-1.30637400	4.30420200
C	-0.67095400	-3.89207200	1.90887500
C	-1.76839700	-2.49945000	3.61155100
C	-0.49769700	-0.94105000	4.99561300
C	-1.88207600	-4.44390200	1.58295900
H	0.21971100	-4.22107900	1.38635700
C	-3.01288500	-3.09581500	3.23584400
C	-1.70331300	-1.54382700	4.62904200
C	-3.07543700	-4.03563500	2.24302000
H	-1.93163700	-5.19323100	0.79985500
H	-3.91265200	-2.77698000	3.75646600
H	-2.61682800	-1.25729500	5.14590800
H	-4.02733700	-4.46136900	1.94093400
C	-1.51937600	1.79358000	-3.85148000
H	-2.37168700	1.13667600	-3.99805500
C	-0.27760600	1.26638100	-3.60961600
H	-0.14927200	0.19039000	-3.57557000
C	-1.71498400	3.20432900	-3.89042700
H	-2.70834200	3.60026900	-4.08051400
C	-0.65679000	4.04752700	-3.68092100
H	-0.79290800	5.12618900	-3.70422600
C	1.92753900	0.31487900	5.68783200
H	2.85447300	0.81781700	5.94651500
C	0.72842500	0.65524900	6.37348200
H	0.75081600	1.40640800	7.15763500
C	-0.44655900	0.04107900	6.03330800
H	-1.37287200	0.29602800	6.54245200
C	1.92642800	-0.63437500	4.69667600
H	2.85531000	-0.88187500	4.19560700
N	2.09437700	0.61443400	1.58726100
S	3.30287100	1.78307400	1.74263100
C	4.89177100	0.76935700	1.72235900
O	3.18966100	2.28233300	3.10603400
O	3.35373600	2.63953000	0.57240800
F	5.85483000	1.53627900	2.23126800
F	4.74964000	-0.32360400	2.47766400
F	5.22006800	0.41182400	0.48336800

H	-5.97883500	3.43465200	2.35187400
H	-4.96519700	0.57817600	1.97439400
C	-1.78085200	4.26331300	1.38894800
C	-1.37776500	4.78699200	2.63152900
C	-0.79074300	4.11937800	0.40430100
C	-0.05097700	5.12870000	2.88541900
H	-2.10938600	4.94063100	3.41929600
C	0.54260700	4.45773900	0.65454500
H	-1.04126200	3.74646200	-0.58307800
C	0.92114300	4.95908500	1.89807100
H	0.22311400	5.52656500	3.85932300
H	1.28351300	4.31826900	-0.12612400
H	1.95894100	5.21071200	2.09581300
C	-4.08675900	5.25860800	1.10126700
H	-5.14542100	5.01673600	0.95179700
H	-4.00620900	5.71932400	2.09679200
C	-3.65892300	6.25896600	0.06061300
H	-2.63332200	6.62300000	0.13212800
C	-4.44653900	6.73076000	-0.91088300
H	-5.47267000	6.36412200	-0.98165400
C	-7.13695100	0.97932000	2.01690100
H	-7.36363100	0.51754800	1.04697500
H	-7.38238300	0.23702300	2.78894800
H	-7.80337100	1.83886500	2.14807800
C	-4.03948400	7.74988200	-1.93685800
H	-4.14820500	7.35499000	-2.95630200
H	-4.67193900	8.64660200	-1.88130700
H	-2.99817400	8.06233600	-1.80240000

INT-13-5

0 imaginary frequency

H = -5315.389046

G = -5315.595688

E(M06-2X-DCM) = -5316.271961

E(M06-2X-cyclohexane) = -5316.245073

C	-1.96034900	4.75083300	0.81566400
C	-2.72590000	4.10155400	2.02222500
H	-2.38250200	3.06656000	2.13173000
H	-2.41765600	4.62411400	2.93641500
C	-4.23014800	4.11907900	1.94666200
C	-2.40207900	4.06615100	-0.50078400
H	-1.86615400	4.49428600	-1.35628300
H	-3.46409400	4.25595300	-0.66077600
N	-2.24058700	2.61539400	-0.49495200

C	-3.07974900	1.74479500	-1.10905300
N	-2.63933000	0.43619100	-1.00505000
C	-3.31590800	-0.75194700	-1.30467200
C	-4.70645800	-0.90374600	-1.16877300
C	-2.54850700	-1.86424900	-1.68036300
C	-5.30000100	-2.13481800	-1.43394900
C	-3.16194900	-3.09108100	-1.93524100
H	-1.47179500	-1.76719900	-1.77157700
C	-4.54291700	-3.23925300	-1.82854300
H	-5.01841100	-4.18791300	-2.04646100
C	-2.31497600	-4.28846100	-2.25311000
C	-6.77596900	-2.31364800	-1.19651200
F	-1.19470100	-3.95847600	-2.93887200
F	-2.97581800	-5.21278900	-2.97802600
F	-1.89375900	-4.91819400	-1.11689000
F	-7.32305900	-3.18752100	-2.07029000
F	-7.45882400	-1.15770300	-1.28940100
F	-7.01622200	-2.81409400	0.04707600
S	-4.47435700	2.21385500	-1.93678100
H	-5.31172500	-0.06261200	-0.86446100
C	-5.00156400	3.03185800	1.85622500
H	-1.65290100	0.31737700	-0.76890400
H	-1.36715400	2.24888300	-0.12746900
H	1.61288500	0.12198300	2.46427500
O	0.57387100	-1.84626000	0.63151300
O	2.56934500	-0.83373100	-0.69093300
P	1.28944100	-0.46213600	0.20319600
O	0.25948900	0.43901000	-0.36446800
C	2.74647100	-4.58817700	2.92556300
C	2.98828300	-4.47764800	1.56025300
C	2.19244100	-3.64674200	0.75256500
C	0.95051100	-2.94265200	2.74360300
C	1.70556300	-3.85437800	3.49759000
C	2.39231400	-1.53572500	-1.90329500
C	2.28916000	-2.92358800	-1.85537600
C	2.00394300	-3.61289300	-3.04555000
C	1.91522900	-2.93519900	-4.25696200
C	2.10951300	-1.55456900	-4.28344500
C	2.33860600	-0.81770500	-3.10991300
H	1.48365100	-3.95991000	4.55535800
H	2.06506500	-1.01737600	-5.22604500
C	2.50450400	-3.92032900	-0.71803600
C	4.00077600	-4.36325800	-0.59940400
H	4.33136400	-4.94676500	-1.46380600

H	4. 63172900	-3. 47048600	-0. 53231700
H	0. 93216500	-5. 48866300	-3. 29544200
H	2. 67664400	-5. 67106500	-3. 10644200
C	1. 25149000	-2. 83120400	1. 37277700
H	3. 35406900	-5. 24349600	3. 54433000
H	1. 69684800	-3. 47242500	-5. 17608600
C	4. 06417200	-5. 14687100	0. 73135300
H	3. 84845200	-6. 21337200	0. 58156200
H	5. 04954000	-5. 09009800	1. 20755900
C	1. 80696500	-5. 08680100	-2. 77502300
C	1. 64683100	-5. 12468800	-1. 24145900
H	1. 95390700	-6. 07542300	-0. 79591100
H	0. 59752900	-4. 95785900	-0. 98217400
C	2. 54520400	0. 66216200	-3. 18685900
C	3. 84369600	1. 19373000	-2. 99688200
C	1. 46093300	1. 51116100	-3. 51355800
C	4. 98553100	0. 37902500	-2. 70971800
C	4. 05288500	2. 61795200	-3. 12106800
C	1. 68751000	2. 93336800	-3. 64157500
C	6. 22930800	0. 92813400	-2. 53969600
H	4. 85896100	-0. 69538000	-2. 63415800
C	5. 36590700	3. 15096200	-2. 93010000
C	2. 97200600	3. 44583400	-3. 43876100
C	6. 42604900	2. 33413200	-2. 64525700
H	7. 07852200	0. 28488500	-2. 32449000
H	5. 50209600	4. 22598400	-3. 02112900
H	3. 13593200	4. 51723700	-3. 53565600
H	7. 41925200	2. 75131200	-2. 50375600
C	-0. 13994600	-2. 13532400	3. 37708100
C	-1. 49065400	-2. 37880300	3. 01941500
C	0. 17434300	-1. 14914400	4. 34653600
C	-1. 87784000	-3. 38094300	2. 07394100
C	-2. 54273100	-1. 59716700	3. 62940200
C	-0. 89212900	-0. 38484500	4. 95784300
C	-3. 19165100	-3. 57192800	1. 73474100
H	-1. 11568500	-3. 99915600	1. 61397100
C	-3. 90064800	-1. 82421800	3. 24192800
C	-2. 21514700	-0. 62752100	4. 58091700
C	-4. 22129600	-2. 77755600	2. 31384100
H	-3. 44718900	-4. 33111300	1. 00284800
H	-4. 67427800	-1. 21314400	3. 70060400
H	-3. 01110300	-0. 04227200	5. 03663500
H	-5. 25066000	-2. 92348900	2. 00120700
C	-0. 90085900	1. 88361600	-4. 02855900

H	-1.90780000	1.49889900	-4.16078200
C	0.12587400	1.03154100	-3.71523100
H	-0.07089600	-0.02943700	-3.61001600
C	-0.66880000	3.28303500	-4.16220400
H	-1.49769100	3.93978100	-4.41013400
C	0.58919800	3.78896100	-3.97206900
H	0.78002500	4.85528300	-4.06781200
C	1.78327700	0.14057100	5.66860200
H	2.81274900	0.36259100	5.93301700
C	0.72757100	0.87567900	6.27607100
H	0.95806000	1.64483000	7.00744000
C	-0.57018000	0.61526900	5.92746600
H	-1.38760700	1.17381500	6.37702900
C	1.51800900	-0.83938000	4.74507200
H	2.33994300	-1.39127200	4.30330900
N	2.12894800	0.07045900	1.58333900
S	3.63507500	0.82407400	1.71115300
C	4.83706800	-0.62409400	1.80950500
O	3.65796400	1.42473400	3.03762200
O	3.96542600	1.54252800	0.49463300
F	5.05864500	-1.14940400	0.60700700
F	5.98107700	-0.15355400	2.30399700
F	4.35602600	-1.56677500	2.62496500
H	-4.71568800	5.09517900	1.99187000
H	-4.52206600	2.05225000	1.81454800
C	-0.44340800	4.65833500	1.06950700
C	0.09412500	5.10682600	2.28994500
C	0.46116500	4.17715000	0.11118500
C	1.46260900	5.06011500	2.54785900
H	-0.56106600	5.50841700	3.05742100
C	1.83479000	4.12369100	0.36559800
H	0.11382300	3.83834100	-0.85903700
C	2.34314200	4.56062100	1.58680500
H	1.84037900	5.41218300	3.50461100
H	2.50267300	3.73019100	-0.39402700
H	3.40908100	4.50856100	1.78817900
C	-2.36235000	6.26546000	0.71240000
H	-3.45392200	6.31553900	0.60238900
H	-2.12004300	6.74434000	1.66874900
C	-1.72676900	7.04783600	-0.40678900
H	-2.05977200	6.81439000	-1.41935400
C	-0.81321000	8.00871800	-0.24309000
H	-0.47983700	8.24827200	0.76830300
C	-6.50066700	3.03469700	1.78483200

H	-6.84229400	2.59293800	0.83955100
H	-6.94353100	2.43842900	2.59456600
H	-6.90570100	4.05043500	1.85038300
C	-0.18470900	8.80472600	-1.35055700
H	-0.57289100	8.50730100	-2.33088900
H	-0.36962100	9.88047700	-1.22521000
H	0.90600400	8.67397300	-1.36275400

INT-13-6

0 imaginary frequency

H = -5315.392682

G = -5315.597255

E(M06-2X-DCM) = -5316.275567

E(M06-2X-cyclohexane) = -5316.250333

C	4.26460600	-2.38930800	0.47241100
C	5.26150500	-3.22217500	1.35205800
H	4.80268900	-3.36216900	2.34064900
H	5.35468700	-4.22571400	0.92185800
C	6.63324800	-2.62791000	1.54485600
C	3.93622400	-1.08281000	1.25352800
H	4.84513600	-0.50807600	1.43369200
H	3.50579800	-1.33852600	2.23175300
N	3.02453300	-0.19776900	0.54904500
C	3.20194500	1.13978800	0.38996500
N	2.09668500	1.73591800	-0.18323300
C	1.87098800	3.09280900	-0.46342300
C	2.84782200	3.93905600	-1.01256500
C	0.58292700	3.59582500	-0.23755200
C	2.53072600	5.26531600	-1.30085200
C	0.28190100	4.92502900	-0.54018500
H	-0.17004300	2.95418000	0.20879800
C	1.25122000	5.77412800	-1.06907300
H	1.01773500	6.80619500	-1.29881000
C	-1.11632800	5.42290500	-0.30824000
C	3.60264400	6.18122600	-1.83291100
F	-1.97334300	4.98782500	-1.26815400
F	-1.19260300	6.76775200	-0.29404800
F	-1.61985600	4.97900700	0.87530000
F	4.26882000	6.80300500	-0.83458200
F	3.08275000	7.15178800	-2.62032500
F	4.51911300	5.51357700	-2.56557800
S	4.59834600	1.96812200	0.85294500
H	3.84098800	3.55939600	-1.20520700
C	7.78036800	-3.25972100	1.27731000

H	1.26883100	1.14413900	-0.25740600
H	2.12856000	-0.59025100	0.26909200
H	-0.58847500	-2.60079400	1.09390200
O	-1.60028600	0.64999500	1.19400500
O	-2.58258300	-0.69766600	-0.77418900
P	-1.31249700	-0.59127900	0.20774100
O	0.04792500	-0.43283000	-0.36184500
C	-4.80213700	0.40139300	3.87139600
C	-5.03316700	0.70399400	2.53422000
C	-3.96084700	0.91389200	1.65212700
C	-2.39309100	0.39620600	3.46118600
C	-3.48842900	0.29663100	4.33287800
C	-2.97047400	0.40608600	-1.56830300
C	-3.77623900	1.39387800	-1.00763200
C	-4.07623800	2.52636100	-1.78546000
C	-3.64659200	2.62489600	-3.10387300
C	-2.90123100	1.58552400	-3.65822600
C	-2.53332400	0.45998200	-2.90479400
H	-3.29633400	0.10283300	5.38393900
H	-2.57106700	1.64286600	-4.69115200
C	-4.48951600	1.48969300	0.34123400
C	-5.91030200	0.83616500	0.31563200
H	-6.60443400	1.37078600	-0.34017000
H	-5.81948500	-0.19267500	-0.05076800
H	-4.49024600	4.55917500	-1.13589500
H	-5.91894800	3.52871300	-1.25050500
C	-2.67443400	0.65865400	2.10771200
H	-5.63217200	0.25142600	4.55692400
H	-3.88163100	3.50469700	-3.69676600
C	-6.35104200	0.82479100	1.79831800
H	-6.88251400	1.74780500	2.06743900
H	-7.02651900	-0.00668300	2.02763100
C	-4.85418500	3.53957700	-0.97892900
C	-4.63102300	3.04777100	0.46369400
H	-5.42860900	3.33818400	1.15334200
H	-3.69191500	3.46304900	0.84344900
C	-1.72546400	-0.62479500	-3.55027200
C	-2.36805400	-1.81274000	-3.97423900
C	-0.34845700	-0.42550200	-3.80734600
C	-3.77423100	-2.03175900	-3.81923500
C	-1.59628600	-2.84834100	-4.62282200
C	0.40822900	-1.46308500	-4.47209700
C	-4.36755600	-3.19102400	-4.24708900
H	-4.37688500	-1.25728200	-3.35763100

C	-2.25157300	-4.04808800	-5.04231100
C	-0.23097500	-2.64781000	-4.84728200
C	-3.59747100	-4.21974900	-4.86047100
H	-5.43810500	-3.32827500	-4.12040000
H	-1.65371200	-4.82000100	-5.52123600
H	0.34407300	-3.42558500	-5.34617700
H	-4.08453300	-5.13342900	-5.18984100
C	-0.98862500	0.26922700	3.96227200
C	-0.13980600	1.40535700	3.94065800
C	-0.51782400	-0.96309300	4.47912100
C	-0.56997500	2.69163300	3.48171700
C	1.22198700	1.28809900	4.41026100
C	0.84386900	-1.06055300	4.95858000
C	0.28266900	3.76494100	3.45948500
H	-1.59475000	2.81898200	3.15171700
C	2.08158000	2.42982100	4.36300600
C	1.67514200	0.06133500	4.90376100
C	1.63066100	3.63464100	3.89702000
H	-0.07407100	4.72256500	3.09237600
H	3.10903200	2.31504600	4.69773900
H	2.70073100	-0.01956400	5.25825200
H	2.29712100	4.49093900	3.85531400
C	1.67549700	0.94232700	-3.72904400
H	2.17505100	1.86401500	-3.44546100
C	0.34575100	0.77389500	-3.44501000
H	-0.19943500	1.56258900	-2.93853000
C	2.41464800	-0.08090000	-4.38926000
H	3.46693200	0.07452300	-4.61058000
C	1.79623900	-1.24943200	-4.74477500
H	2.34690600	-2.03659000	-5.25470200
C	-0.83241000	-3.32519900	5.03196100
H	-1.46825800	-4.20546300	5.04882700
C	0.50536100	-3.41179200	5.51259000
H	0.87585400	-4.35310800	5.90941900
C	1.31628000	-2.30908100	5.47325200
H	2.33956300	-2.35892100	5.83858500
C	-1.32439300	-2.14571600	4.53545600
H	-2.34487300	-2.10258200	4.17325800
N	-1.46846100	-2.08470200	0.99328500
S	-2.80016900	-3.08737300	1.26270200
C	-3.30284000	-3.72712300	-0.45163600
O	-3.92711500	-2.30375700	1.74288800
O	-2.27348300	-4.24580900	1.97314100
F	-2.26297500	-3.69652900	-1.28231400

F	-3.71171800	-4.98544200	-0.29641300
F	-4.30015300	-2.99212900	-0.92719300
H	6.68411200	-1.62174300	1.96352200
H	7.74010800	-4.27191800	0.86859200
C	2.96500800	-3.20209000	0.30134000
C	2.29147700	-3.69621600	1.43501600
C	2.38166500	-3.45372000	-0.94999400
C	1.11439500	-4.43821100	1.32325100
H	2.68162900	-3.50557500	2.43039400
C	1.20209800	-4.19287000	-1.06985000
H	2.84997700	-3.08082100	-1.85066900
C	0.56808300	-4.70133100	0.06267000
H	0.62415800	-4.80929100	2.21903100
H	0.77790300	-4.36257800	-2.05578800
H	-0.34250100	-5.28610800	-0.02668100
C	4.93894900	-1.98303100	-0.87142400
H	4.23948800	-1.38716100	-1.46799100
H	5.75524900	-1.29797800	-0.60339600
C	5.52082800	-3.08710300	-1.71679300
H	6.20047100	-3.77712800	-1.21716300
C	5.32519400	-3.23114500	-3.03097700
H	4.65740600	-2.53378200	-3.54246700
C	9.15371900	-2.69486500	1.50239200
H	9.10913100	-1.67944900	1.91008800
H	9.73121100	-3.31680400	2.20003900
H	9.72714600	-2.65955200	0.56621300
C	5.96194200	-4.28600900	-3.89077100
H	6.61347100	-4.94243100	-3.30379000
H	5.20582000	-4.91311500	-4.38327400
H	6.56675600	-3.83838900	-4.69147000

INT-13-7

0 imaginary frequency

H = -5315.384581

G = -5315.590667

E(M06-2X-DCM) = -5316.264348

E(M06-2X-cyclohexane) = -5316.239602

C	-4.89087700	-0.67830300	-0.99787500
C	-6.21465800	-0.91068400	-1.80599600
H	-5.95815700	-1.06397500	-2.86241400
H	-6.66407500	-1.84782700	-1.45911400
C	-7.24032100	0.19232500	-1.73566700
C	-4.18642000	0.57281300	-1.59845400
H	-4.85621500	1.43181900	-1.57269600

H	-3.94221400	0.37906000	-2.65294000
N	-2.98432700	0.97403600	-0.88393800
C	-2.65108200	2.26533600	-0.60560000
N	-1.43623900	2.35070600	0.04265900
C	-0.67486700	3.43625300	0.49382000
C	-1.01149800	4.79366600	0.35720000
C	0.53503600	3.10971700	1.13428500
C	-0.15274800	5.77448300	0.85375300
C	1.36859000	4.10482700	1.63442800
H	0.82202300	2.06930000	1.23540100
C	1.03712300	5.45312700	1.50299500
H	1.68253900	6.22692900	1.89989100
C	2.67947700	3.72033700	2.25681800
C	-0.48190100	7.22349400	0.60699200
F	3.66460800	3.58734100	1.32357900
F	2.60991300	2.53208800	2.90343000
F	3.11596000	4.63779300	3.14385900
F	0.05604400	7.65636200	-0.56428900
F	0.01470000	8.02482200	1.57679400
F	-1.80787100	7.44606600	0.53356300
S	-3.64331100	3.57027600	-1.01431000
H	-1.93574800	5.06835200	-0.12902900
C	-8.49179400	0.04097700	-1.29203800
H	-0.98680200	1.45172500	0.21892800
H	-2.30367200	0.24746200	-0.67658400
H	-0.00323900	-2.48337600	-1.48751300
O	2.03014400	0.07852200	-0.48950800
O	1.73549600	-1.85837500	1.18753600
P	1.01463900	-1.07309700	-0.00607000
O	-0.32373600	-0.46929600	0.20675300
C	5.45903000	-1.08622300	-2.56827300
C	5.39889200	-1.24030800	-1.18758100
C	4.31461700	-0.72627200	-0.45588700
C	3.28457000	0.03041100	-2.54870000
C	4.43172700	-0.40685200	-3.22862500
C	2.34887500	-1.24765300	2.29650700
C	3.64018000	-0.74284600	2.17777500
C	4.19855600	-0.10099400	3.29803700
C	3.52795400	-0.06222100	4.51493500
C	2.25914000	-0.63119800	4.61475000
C	1.63037900	-1.21299800	3.50445400
H	4.49868900	-0.22782900	-4.29764600
H	1.72005600	-0.60160000	5.55692200
C	4.65609000	-0.75757400	1.03391000

C	5.59491800	-2.00749400	1.07159700
H	6.24642400	-2.01101100	1.95075600
H	4.98058200	-2.91251400	1.09653800
H	5.61788000	1.54491900	3.35475600
H	6.36723600	-0.05151900	3.33429000
C	3.23406000	-0.21177500	-1.16188400
H	6.30431200	-1.47284400	-3.13192000
H	3.97527200	0.42791700	5.37562100
C	6.37386300	-1.93985500	-0.26364500
H	7.30810900	-1.37142000	-0.15949200
H	6.64913000	-2.93288900	-0.63595700
C	5.52308000	0.53383000	2.94428800
C	5.48554700	0.52339000	1.40395500
H	6.47672400	0.52392400	0.94171300
H	4.94767800	1.40965600	1.05260700
C	0.23653300	-1.74505100	3.61883000
C	0.01055600	-3.14143300	3.64339400
C	-0.84554000	-0.83911200	3.72651800
C	1.07082100	-4.10007400	3.56508900
C	-1.33995200	-3.64105800	3.76646400
C	-2.19176600	-1.35292000	3.84775400
C	0.81693900	-5.44632600	3.58959900
H	2.09319800	-3.74630900	3.48751900
C	-1.56100900	-5.05405200	3.78911800
C	-2.40099700	-2.73522300	3.86410300
C	-0.51618800	-5.93392900	3.70012600
H	1.64013100	-6.15222400	3.52356700
H	-2.58328800	-5.41338800	3.88108400
H	-3.41625200	-3.11558800	3.95809900
H	-0.69741900	-7.00504500	3.71644600
C	2.19964200	0.78097900	-3.26006700
C	2.01108400	2.15825000	-2.97485000
C	1.39916500	0.14433200	-4.23969200
C	2.82572200	2.88384700	-2.04797000
C	0.96554100	2.89083600	-3.65366700
C	0.36713800	0.89455400	-4.92066500
C	2.60744000	4.21271300	-1.79209100
H	3.63577000	2.37111400	-1.54209500
C	0.76124500	4.27208500	-3.34577700
C	0.17159400	2.23976800	-4.60147300
C	1.55400500	4.91944500	-2.43741800
H	3.23700700	4.72778900	-1.07333800
H	-0.04793200	4.79554600	-3.84861400
H	-0.61520800	2.79703100	-5.10536800

H	1. 37139500	5. 96067900	-2. 18998600
C	-1. 75147800	1. 42971500	3. 79714900
H	-1. 59503200	2. 50439000	3. 77164900
C	-0. 67659100	0. 58404100	3. 70450200
H	0. 32184100	0. 99699600	3. 61205300
C	-3. 07516200	0. 91798600	3. 91545800
H	-3. 91352900	1. 60564700	3. 97992400
C	-3. 28532000	-0. 43467100	3. 94018200
H	-4. 29236300	-0. 83770600	4. 01536600
C	0. 76434900	-1. 82249800	-5. 54648200
H	0. 90729600	-2. 87183700	-5. 78947700
C	-0. 24561000	-1. 07714700	-6. 21846700
H	-0. 86032400	-1. 55942200	-6. 97359600
C	-0. 43631700	0. 24202000	-5. 90778000
H	-1. 20507400	0. 82501900	-6. 40940800
C	1. 55302000	-1. 23384500	-4. 59228400
H	2. 31524500	-1. 81308900	-4. 08967800
N	0. 95092100	-2. 36621600	-1. 13162200
S	1. 67901900	-3. 90011800	-0. 89696600
C	1. 72367000	-4. 50549600	-2. 67856300
O	0. 76458500	-4. 80682300	-0. 21474000
O	3. 06303500	-3. 72756100	-0. 48627900
F	0. 58277600	-4. 19641500	-3. 30332000
F	2. 75359100	-3. 97154900	-3. 32883800
F	1. 86421800	-5. 82757900	-2. 63919300
H	-6. 94345900	1. 17049100	-2. 11676000
H	-8. 80010500	-0. 93562800	-0. 91527200
C	-3. 95755200	-1. 89532900	-1. 17847600
C	-3. 73133500	-2. 42956200	-2. 46181900
C	-3. 25631900	-2. 47995800	-0. 11167300
C	-2. 87909900	-3. 51288800	-2. 66539600
H	-4. 22404800	-1. 99608400	-3. 32619900
C	-2. 40320200	-3. 57050200	-0. 30688100
H	-3. 36298600	-2. 09228000	0. 89443000
C	-2. 21727100	-4. 10046100	-1. 58394800
H	-2. 73722400	-3. 90159000	-3. 67065000
H	-1. 88498200	-4. 00491000	0. 54298800
H	-1. 57003900	-4. 95962400	-1. 72947300
C	-5. 24334200	-0. 38831100	0. 48865900
H	-4. 31537600	-0. 19258300	1. 04139300
H	-5. 80569300	0. 55155000	0. 51818800
C	-6. 04124900	-1. 45623200	1. 19517500
H	-5. 67241500	-2. 48011100	1. 12296900
C	-7. 14553700	-1. 23029800	1. 91465200

H	-7.52822600	-0.21049000	1.98379400
C	-9.53630600	1.12012300	-1.26804100
H	-10.41074600	0.84243000	-1.87260800
H	-9.90515000	1.29467500	-0.24799800
H	-9.14543900	2.06809400	-1.65282500
C	-7.92856700	-2.28094100	2.65064600
H	-8.96642000	-2.32895700	2.29314900
H	-7.48354600	-3.27464900	2.52849700
H	-7.98096400	-2.06272300	3.72624300

INT-13-8

0 imaginary frequency

H = -5315.392640

G = -5315.595469

E(M06-2X-DCM) = -5316.271694

E(M06-2X-cyclohexane) = -5316.246935

C	3.50292100	-3.84311700	-0.66167700
C	4.91503800	-3.55227200	-0.06644800
H	5.14490500	-4.31575800	0.68558400
H	5.61979700	-3.73613600	-0.89191800
C	5.22185400	-2.18550400	0.49062800
C	3.16325000	-2.84041300	-1.80564200
H	2.39382000	-3.27653900	-2.45622700
H	4.04839600	-2.67394800	-2.42228900
N	2.69623100	-1.53308500	-1.36548000
C	3.13373400	-0.33978700	-1.84223500
N	2.33998900	0.70677800	-1.41712400
C	2.52438400	2.08824000	-1.56837500
C	3.78438400	2.70847700	-1.56980400
C	1.37535500	2.88794700	-1.64835500
C	3.87384100	4.09389000	-1.68073400
C	1.48560900	4.27435200	-1.75275600
H	0.39508500	2.42328800	-1.62792500
C	2.73350900	4.89254600	-1.78331200
H	2.81798800	5.96789400	-1.88353700
C	0.24152000	5.11481700	-1.75313800
C	5.22145400	4.76016300	-1.59126700
F	-0.79643900	4.49493000	-2.36410200
F	0.42047600	6.30266700	-2.36408300
F	-0.17491600	5.39089100	-0.48334400
F	6.22512400	3.94785000	-1.97056600
F	5.49130100	5.15270000	-0.31659600
F	5.28136800	5.87414800	-2.35438800
S	4.48036800	-0.16882000	-2.84920000

H	4.67980800	2.10963200	-1.49128500
C	5.77248900	-1.96725300	1.68911000
H	1.42763200	0.44069700	-1.04324400
H	1.83046100	-1.53000300	-0.83266100
H	-0.92330800	-1.93147200	1.69958100
O	-1.12527400	1.35166100	0.92986900
O	-2.83345500	-0.10829700	-0.35590000
P	-1.37687100	-0.12096000	0.33076200
O	-0.19753000	-0.51354300	-0.47832100
C	-3.63117900	2.79569000	3.95695200
C	-4.06330900	2.78717200	2.63586600
C	-3.19028400	2.42040800	1.59903600
C	-1.44677100	1.95066800	3.25301500
C	-2.31834500	2.42395900	4.24738200
C	-3.12145300	0.80166400	-1.40029500
C	-3.49051400	2.10496300	-1.07634800
C	-3.67018500	3.02650100	-2.12276300
C	-3.56781500	2.62984300	-3.45113800
C	-3.27845800	1.29829700	-3.74408900
C	-3.03481600	0.35559000	-2.73252200
H	-1.95690100	2.46618400	5.27035300
H	-3.21497800	0.96969600	-4.77710500
C	-3.83073300	2.76721500	0.25751500
C	-5.34117400	2.59848200	0.62791200
H	-6.00198400	3.12979300	-0.06401000
H	-5.59710400	1.53336900	0.59254900
H	-3.36876800	5.17896500	-2.09924800
H	-5.00805300	4.67196700	-1.68790600
C	-1.93838600	1.91827200	1.93452100
H	-4.30226100	3.09375900	4.75832100
H	-3.70977000	3.34733300	-4.25493200
C	-5.43541900	3.10967300	2.08372900
H	-5.64305300	4.18782900	2.11960600
H	-6.23251000	2.61596900	2.65050400
C	-3.94676100	4.40867300	-1.57915700
C	-3.54364000	4.26780300	-0.09859000
H	-4.07297000	4.95787100	0.56451400
H	-2.47191800	4.46173600	0.00473000
C	-2.73007000	-1.06057700	-3.11571900
C	-3.74351400	-2.04386000	-3.01057100
C	-1.47157900	-1.38790800	-3.67357100
C	-5.06754800	-1.74855700	-2.55364200
C	-3.46263200	-3.40297900	-3.41405200
C	-1.21184500	-2.74737400	-4.09351500

C	-6.02915700	-2.72221200	-2.47326800
H	-5.30937100	-0.72940800	-2.27260100
C	-4.48845900	-4.39225400	-3.29773800
C	-2.20442900	-3.71788600	-3.93498600
C	-5.73683000	-4.06654400	-2.83999500
H	-7.02743000	-2.46767200	-2.12738300
H	-4.25540900	-5.41182800	-3.59566800
H	-2.00105100	-4.74028600	-4.24758700
H	-6.51020700	-4.82593800	-2.76427000
C	-0.05123000	1.54272100	3.60911100
C	1.04429500	2.31114300	3.13878200
C	0.17049700	0.43818600	4.46971700
C	0.88814000	3.47378200	2.31836400
C	2.39020200	1.93890800	3.51308100
C	1.52216000	0.09056100	4.84963300
C	1.97114800	4.18808600	1.87732700
H	-0.10861800	3.79893300	2.04367200
C	3.49356400	2.70296900	3.01849300
C	2.59042800	0.84342400	4.35692500
C	3.29633300	3.79379900	2.21601200
H	1.81392400	5.06064500	1.25196600
H	4.49793400	2.39210700	3.29578900
H	3.60531000	0.57350900	4.64216700
H	4.13957300	4.35401900	1.82348900
C	0.76797400	-0.76868400	-4.43439900
H	1.54677800	-0.02291500	-4.56240100
C	-0.42782300	-0.42462500	-3.86057100
H	-0.59820100	0.59864900	-3.54552400
C	1.01503400	-2.10829800	-4.85213400
H	1.97102600	-2.35785000	-5.30323000
C	0.05376200	-3.06761800	-4.67913300
H	0.22803700	-4.09312500	-4.99704100
C	-0.63814900	-1.43831300	5.81533300
H	-1.46503800	-2.04282500	6.17631400
C	0.69363300	-1.76453500	6.19887500
H	0.87270100	-2.60325500	6.86628000
C	1.74027600	-1.02039500	5.72378100
H	2.76363600	-1.25763400	6.00546000
C	-0.88926200	-0.37725000	4.98439100
H	-1.91097500	-0.14817400	4.70585600
N	-1.68011100	-1.25533800	1.55458100
S	-3.09772500	-1.72621000	2.33909900
C	-4.11981000	-2.63292000	1.02616700
O	-3.87718600	-0.55760000	2.71471500

O	-2.69051600	-2.75373500	3.28937700
F	-4.99475500	-1.79537200	0.48638500
F	-3.32125000	-3.14269900	0.08797200
F	-4.76829500	-3.61858900	1.64279600
H	5.05808200	-1.33826000	-0.17213700
H	5.96875600	-2.81933600	2.34517900
C	2.36802100	-3.88491500	0.37673600
C	2.58829800	-3.72273500	1.75305600
C	1.04696600	-4.12875800	-0.04215700
C	1.54158000	-3.81028400	2.67260100
H	3.58389300	-3.50604000	2.11656400
C	-0.00176500	-4.22906400	0.87316600
H	0.82344400	-4.24983100	-1.09871000
C	0.24006800	-4.07354800	2.24215900
H	1.74319400	-3.66538800	3.73029500
H	-1.00816600	-4.42831700	0.51413000
H	-0.57156000	-4.15667400	2.95882800
C	3.59315100	-5.24599200	-1.36467200
H	2.62331000	-5.44894100	-1.84040400
H	4.32836600	-5.17579400	-2.17764800
C	3.94557700	-6.39920000	-0.46607900
H	3.26485100	-6.58600300	0.36588600
C	5.00147200	-7.20189500	-0.62985200
H	5.68110400	-7.01327300	-1.46352100
C	6.17027000	-0.62104100	2.22456400
H	5.93657500	0.17746800	1.51272300
H	5.65180400	-0.39743500	3.16769600
H	7.24655100	-0.57864100	2.44154800
C	5.34251500	-8.37372700	0.24592100
H	5.36347700	-9.30907400	-0.33002600
H	6.33948000	-8.26018800	0.69305600
H	4.61793200	-8.49311300	1.05859800

INT-13-9

0 imaginary frequency

H = -5315.393669

G = -5315.597163

E(M06-2X-DCM) = -5316.278327

E(M06-2X-cyclohexane) = -5316.254011

C	-1.42473800	4.62299900	0.74366700
C	-2.31023600	4.08023200	1.91607000
H	-2.09842300	3.01435100	2.05787600
H	-1.99462400	4.58815100	2.83737600
C	-3.79719800	4.26965000	1.76696600

C	-1.95875800	4.07388900	-0.60196400
H	-1.42309100	4.51967400	-1.44772800
H	-3.00589000	4.35751500	-0.71372000
N	-1.90108600	2.62035100	-0.66913500
C	-2.81000400	1.83978200	-1.30262300
N	-2.49333900	0.49554100	-1.20434200
C	-3.25427900	-0.64110400	-1.49721600
C	-4.65915800	-0.66130100	-1.52928700
C	-2.55975900	-1.84617300	-1.69080100
C	-5.33135700	-1.85746700	-1.76878500
C	-3.25260200	-3.03313400	-1.92330900
H	-1.47539700	-1.85482900	-1.64707300
C	-4.64492500	-3.05412400	-1.97609800
H	-5.18017200	-3.97517900	-2.17135900
C	-2.48934300	-4.32131000	-2.02700600
C	-6.83534800	-1.88085400	-1.69629300
F	-3.15746300	-5.26549700	-2.71879200
F	-2.23584200	-4.84927900	-0.79476300
F	-1.28389100	-4.15750700	-2.62318000
F	-7.38686300	-0.70122000	-2.03749400
F	-7.26031200	-2.16353100	-0.43457400
F	-7.36391700	-2.83024600	-2.49997100
S	-4.13686700	2.45569400	-2.14652100
H	-5.21239800	0.25288100	-1.37274100
C	-4.68269600	3.27427600	1.66360700
H	-1.54486300	0.29800200	-0.88454000
H	-1.05138400	2.17642100	-0.32887700
H	1.78715600	1.28716100	1.83099100
O	0.39889500	-1.66485300	0.84858200
O	2.55149400	-1.03477000	-0.42818400
P	1.28261200	-0.41678300	0.34536800
O	0.38692000	0.53710200	-0.35232500
C	2.00437400	-4.26554300	3.70145900
C	2.39000900	-4.36725500	2.36968400
C	1.76607900	-3.58802300	1.38186800
C	0.42435300	-2.49586000	3.11565200
C	0.99553700	-3.36745100	4.05557600
C	2.37703700	-1.90970400	-1.52433800
C	2.15175500	-3.26250000	-1.28136100
C	1.89395200	-4.09976500	-2.38132500
C	1.93887300	-3.60996600	-3.68159900
C	2.24045000	-2.26561500	-3.89479300
C	2.45495200	-1.38112400	-2.82660300
H	0.65931200	-3.30794300	5.08642800

H	2.29618700	-1.87349900	-4.90593700
C	2.18550600	-4.09150400	0.00300400
C	3.61932900	-4.62001800	0.33651400
H	3.98205400	-5.33886600	-0.40478500
H	4.31337000	-3.77215200	0.35749700
H	0.70211500	-5.91615800	-2.46074700
H	2.40541900	-6.18175300	-2.08340700
C	0.87328900	-2.60433800	1.78630800
H	2.47836700	-4.87819100	4.46395000
H	1.73744100	-4.26455000	-4.52535900
C	3.48274200	-5.21777900	1.75672400
H	3.20031900	-6.27877900	1.72183100
H	4.41620100	-5.15816600	2.32708100
C	1.55906000	-5.49954200	-1.92257100
C	1.27156900	-5.29377700	-0.42315400
H	1.45452000	-6.18617100	0.18199700
H	0.22301900	-5.01073700	-0.29183200
C	2.78599700	0.05276300	-3.11204000
C	4.13409500	0.47897400	-3.04049800
C	1.77215000	0.94995900	-3.52279700
C	5.21131800	-0.40526800	-2.71256800
C	4.46326000	1.85475700	-3.33619200
C	2.11593200	2.32307500	-3.81988000
C	6.50754600	0.03750700	-2.65921600
H	4.98999500	-1.44724200	-2.50914700
C	5.82676300	2.27853600	-3.25801000
C	3.44576000	2.73864200	-3.70856300
C	6.82319700	1.39972400	-2.92807100
H	7.30576400	-0.65736500	-2.41223400
H	6.05519000	3.31890200	-3.47757000
H	3.69892900	3.77230400	-3.93702500
H	7.85607500	1.73323400	-2.87822900
C	-0.63758700	-1.51819400	3.51313000
C	-1.96146000	-1.69660500	3.03682100
C	-0.33145400	-0.44055200	4.38058400
C	-2.34827100	-2.79338600	2.20205800
C	-2.98832300	-0.74984600	3.40948400
C	-1.37223500	0.49361400	4.75129900
C	-3.63451600	-2.92804500	1.74883800
H	-1.60719800	-3.53450100	1.92523100
C	-4.31670100	-0.92233800	2.90714300
C	-2.66537000	0.31825200	4.25158500
C	-4.63514600	-1.97559200	2.09273000
H	-3.88883700	-3.76670300	1.10860000

H	-5.07074500	-0.19130700	3.18934600
H	-3.44104300	1.03047100	4.52558100
H	-5.63922300	-2.08494200	1.69408000
C	-0.55557500	1.45786500	-4.07067700
H	-1.59072500	1.14430800	-4.16613000
C	0.40058900	0.56313600	-3.66715200
H	0.12201400	-0.46312300	-3.45487600
C	-0.21247700	2.81181100	-4.35145000
H	-0.98922200	3.50477000	-4.66139000
C	1.08591300	3.22798600	-4.22922900
H	1.36311500	4.25637500	-4.44976700
C	1.24581500	0.85322500	5.73030900
H	2.25587300	1.00608000	6.09883200
C	0.21496600	1.76421500	6.09822200
H	0.44165700	2.59646900	6.75915800
C	-1.05513000	1.58607400	5.61888500
H	-1.85340500	2.27262100	5.89124800
C	0.98169400	-0.20868400	4.90447800
H	1.78113000	-0.88936800	4.63625000
N	2.11265500	0.34077600	1.61515100
S	3.61600200	0.03272000	2.32225100
C	4.90044800	0.42515800	0.97990500
O	3.75608200	-1.38795900	2.59985000
O	3.78280700	1.06329200	3.33897300
F	5.94834200	0.97561200	1.59174600
F	5.27634100	-0.69787300	0.38086400
F	4.40325900	1.28304900	0.09242500
C	0.05785900	4.25832300	0.97116500
C	0.57752500	4.03662600	2.25897700
C	0.96496600	4.19160400	-0.10305700
C	1.93719800	3.78891200	2.46773700
H	-0.07333300	4.05227300	3.12521800
C	2.32342700	3.94333100	0.09834000
H	0.61576500	4.32849800	-1.12064300
C	2.82119000	3.75187800	1.38740900
H	2.30260700	3.61922200	3.47646600
H	2.98790900	3.88723500	-0.75938900
H	3.87738200	3.56076300	1.55099000
C	-1.56704000	6.18770700	0.71344700
H	-2.62944700	6.42999500	0.59283700
H	-1.26908900	6.55251100	1.70731100
C	-0.78094600	6.92750900	-0.33578600
C	-1.32309800	7.63586900	-1.33184500
C	-6.16641100	3.44590200	1.51768100

H	-6.50954500	3.02453800	0.56378000
H	-6.71298700	2.92179300	2.31380500
H	-6.45560400	4.50212700	1.54583400
C	-0.55300000	8.40715100	-2.36532400
H	-0.80960500	9.47499300	-2.33802700
H	0.52805500	8.31545600	-2.21402800
H	-0.78677300	8.05653600	-3.37981800
H	-2.41090400	7.67558500	-1.41785200
H	-4.31703400	2.24587300	1.66490400
H	-4.16852200	5.29572900	1.76675500
H	0.30511000	6.89203900	-0.24752200

TS-EF-4SS

1 imaginary frequency

H = -5315.358666

G = -5315.559033

E(M06-2X-DCM) = -5316.244184

E(M06-2X-cyclohexane) = -5316.215057

O	-0.62458400	-2.65787900	-0.77408300
O	-2.62893400	-1.12694100	-0.16036000
P	-0.99127600	-1.18827800	-0.15324700
O	-0.50785100	-0.06981500	-1.02906100
C	-1.75630600	-3.30351300	-4.75338100
C	-2.65188700	-3.52509000	-3.71219200
C	-2.24221100	-3.38001800	-2.37903900
C	-0.02159800	-2.69774200	-3.13200800
C	-0.44803400	-2.92369200	-4.45280900
C	-3.36582900	-2.08420200	0.53981700
C	-3.56515700	-3.34699100	-0.02162400
C	-4.15933900	-4.35325800	0.75751800
C	-4.65009300	-4.07555100	2.02828100
C	-4.55566700	-2.77419900	2.51882500
C	-3.90900400	-1.75646200	1.79843300
H	0.26680000	-2.77068900	-5.25602200
H	-4.97200400	-2.53093300	3.49197500
C	-3.33608700	-3.87141700	-1.43917900
C	-4.59714200	-3.63169400	-2.33826200
H	-4.89647800	-2.58089800	-2.24969000
H	-5.44941200	-4.24850500	-2.03651900
H	-5.15732200	-5.93343100	-0.34243600
H	-3.82591100	-6.50587000	0.65685900
C	-0.96010200	-2.91199300	-2.10431100
H	-2.06409600	-3.42640100	-5.78883300
H	-5.11268000	-4.85443800	2.62912200

C	-4. 11284200	-3. 91412400	-3. 77769800
H	-4. 66748500	-3. 34169100	-4. 53005300
H	-4. 23174600	-4. 97503200	-4. 03921300
C	-4. 15277100	-5. 67507100	0. 02118800
C	-3. 18302400	-5. 40176400	-1. 14757300
H	-2. 15306400	-5. 59618400	-0. 82743500
H	-3. 38044300	-6. 01665000	-2. 03121300
C	-3. 89672400	-0. 37520900	2. 37965300
C	-3. 16552300	-0. 10643200	3. 56244400
C	-4. 73244100	0. 62421000	1. 81925000
C	-2. 29109500	-1. 06762100	4. 16332400
C	-3. 28413500	1. 18590600	4. 20134400
C	-4. 82928300	1. 91781000	2. 45949200
C	-1. 60598900	-0. 78488600	5. 31487400
H	-2. 14391300	-2. 01875200	3. 66951200
C	-2. 56357800	1. 43471400	5. 41237100
C	-4. 10614000	2. 16223100	3. 63125300
C	-1. 75166500	0. 47704900	5. 95798500
H	-0. 92561800	-1. 52301100	5. 72827900
H	-2. 68137200	2. 40420000	5. 89171100
H	-4. 20235500	3. 12892400	4. 12282100
H	-1. 20717000	0. 67796400	6. 87673500
C	1. 38942300	-2. 26672700	-2. 88302700
C	1. 84600300	-1. 02567100	-3. 39325100
C	2. 28984600	-3. 13238900	-2. 21377600
C	0. 98150400	-0. 08224700	-4. 03972400
C	3. 23916800	-0. 66467500	-3. 25593300
C	3. 67033800	-2. 73775200	-2. 04765700
C	1. 46077000	1. 09720000	-4. 54948100
H	-0. 07484100	-0. 31157900	-4. 11328600
C	3. 70319400	0. 56890200	-3. 81600000
C	4. 11033700	-1. 52286100	-2. 57966500
C	2. 84361200	1. 42621400	-4. 44951900
H	0. 78016600	1. 78919000	-5. 03940900
H	4. 76093000	0. 80483900	-3. 72598300
H	5. 15242500	-1. 23365300	-2. 46111600
H	3. 20972000	2. 35648200	-4. 87602400
C	-6. 34843800	1. 38263400	0. 14478700
H	-6. 94503000	1. 18305200	-0. 74107400
C	-5. 53243100	0. 40436300	0. 65149200
H	-5. 49213700	-0. 56381200	0. 16606000
C	-6. 42967000	2. 65868000	0. 77208800
H	-7. 09085800	3. 41893200	0. 36452100
C	-5. 69007800	2. 91379400	1. 89716300

H	-5.76138500	3.87542900	2.40134400
C	2.79729500	-5.22182400	-1.05246200
H	2.47291700	-6.18634900	-0.67111000
C	4.14946500	-4.81604900	-0.86994400
H	4.84231100	-5.46935200	-0.34666400
C	4.57023500	-3.61005600	-1.35983100
H	5.60212400	-3.28983200	-1.23728200
C	1.90370900	-4.41280000	-1.70359500
H	0.88137100	-4.74549600	-1.83973300
C	-1.82056800	3.78010100	-0.77838900
C	-1.79183500	4.11636000	0.75687500
H	-1.50078500	5.16421200	0.89062600
H	-2.81996100	4.01810400	1.13726500
C	-0.94563800	3.25629600	1.62463100
C	-0.36469100	3.58253800	-1.26040300
H	0.21025100	4.49948700	-1.12921700
H	-0.36783000	3.32551900	-2.32550200
N	0.34823100	2.51090200	-0.55430600
C	1.63438100	2.59330000	-0.14284400
N	2.31722900	1.44415000	-0.00429100
C	3.68811900	1.35533900	0.40618500
C	4.68184700	1.68090300	-0.51329000
C	4.02087100	0.87044100	1.67166500
C	6.02370300	1.51500000	-0.16888000
C	5.36781800	0.72499800	2.00850200
H	3.23962000	0.58774100	2.36846700
C	6.37385000	1.04005000	1.09336200
H	7.41538900	0.90438600	1.35770500
C	5.73847200	0.26429600	3.39549100
C	7.06868900	1.78587600	-1.21590800
F	6.95287900	-0.33069500	3.41591200
F	4.84383900	-0.61055000	3.89034500
F	5.79742900	1.30587600	4.25911400
F	7.02156900	0.85409900	-2.20806600
F	8.31893700	1.76628700	-0.71517700
F	6.88153100	2.98313200	-1.81194200
S	2.29754400	4.10445300	0.38250100
H	4.40242400	2.03348000	-1.49968800
H	1.85688100	0.54595100	-0.18463600
H	0.00563700	1.55021100	-0.75419200
C	0.03711600	3.79164500	2.46410100
H	-0.09461300	4.85912900	2.68025400
H	0.95417200	3.98171400	1.57847500
N	-0.57708900	-1.23871800	1.40688600

S	0.92847100	-1.36031100	1.89527400
O	1.17946300	-0.51392500	3.07489600
O	1.93117900	-1.30753600	0.80460500
C	1.03868600	-3.10704400	2.55233100
F	0.76508000	-3.98926700	1.58846300
F	0.16512600	-3.28110400	3.55749800
F	2.27177200	-3.33150600	3.01522800
H	-1.11227900	2.18064400	1.62434700
C	0.66578500	2.97174300	3.58139800
H	0.77934700	1.91970200	3.30262400
H	1.65104200	3.37015000	3.84284500
H	0.03645500	3.00797300	4.47732100
C	-2.46634800	4.98228400	-1.49533700
C	-3.75902700	5.39275900	-1.12393200
C	-1.82507100	5.70867000	-2.50888000
C	-4.37994000	6.48151500	-1.73281500
H	-4.29932100	4.85255700	-0.35122100
C	-2.44582800	6.79948300	-3.12384800
H	-0.83082900	5.43538100	-2.84362800
C	-3.72470100	7.19380100	-2.73892200
H	-5.37934100	6.77253400	-1.41974500
H	-1.92020000	7.33865500	-3.90752600
H	-4.20652600	8.04292600	-3.21572700
C	-2.68381900	2.49865200	-1.02923500
H	-3.70606000	2.71293000	-0.70388400
H	-2.32301600	1.68649800	-0.38984500
C	-2.69606500	2.01088100	-2.45624900
H	-1.84978300	1.39629600	-2.76178500
C	-3.67563700	2.25101000	-3.33288600
H	-4.53296500	2.84725600	-3.01584400
C	-3.70460700	1.75633000	-4.75065700
H	-4.59228300	1.13682800	-4.93876100
H	-3.75027700	2.59145000	-5.46323000
H	-2.81902200	1.15599100	-4.98565700

TS-EF-4SS-1

l imaginary frequency

H = -5315.358665

G = -5315.559033

E(M06-2X-DCM) = -5316.244184

E(M06-2X-cyclohexane) = -5316.215057

O	-0.62458500	-2.65787800	-0.77408500
O	-2.62893500	-1.12694000	-0.16036000
P	-0.99127700	-1.18827800	-0.15324800

O	-0.50785200	-0.06981400	-1.02906100
C	-1.75630900	-3.30350800	-4.75338400
C	-2.65189000	-3.52508600	-3.71219500
C	-2.24221300	-3.38001400	-2.37904100
C	-0.02160000	-2.69773800	-3.13201100
C	-0.44803600	-2.92368700	-4.45281200
C	-3.36582900	-2.08420200	0.53981600
C	-3.56515800	-3.34699000	-0.02162600
C	-4.15934000	-4.35325800	0.75751500
C	-4.65009400	-4.07555200	2.02827800
C	-4.55566800	-2.77420100	2.51882400
C	-3.90900400	-1.75646300	1.79843200
H	0.26679700	-2.77068300	-5.25602500
H	-4.97200400	-2.53093600	3.49197400
C	-3.33608800	-3.87141500	-1.43918200
C	-4.59714400	-3.63169100	-2.33826400
H	-4.89648000	-2.58089500	-2.24969200
H	-5.44941400	-4.24850200	-2.03652200
H	-5.15732300	-5.93342900	-0.34244100
H	-3.82591200	-6.50587000	0.65685300
C	-0.96010400	-2.91199000	-2.10431400
H	-2.06409800	-3.42639500	-5.78883500
H	-5.11268000	-4.85443900	2.62911800
C	-4.11284400	-3.91412000	-3.77770100
H	-4.66748800	-3.34168600	-4.53005500
H	-4.23174900	-4.97502700	-4.03921700
C	-4.15277200	-5.67507000	0.02118300
C	-3.18302600	-5.40176200	-1.14757700
H	-2.15306600	-5.59618200	-0.82743900
H	-3.38044500	-6.01664700	-2.03121800
C	-3.89672300	-0.37521100	2.37965400
C	-3.16552200	-0.10643500	3.56244500
C	-4.73243900	0.62421000	1.81925200
C	-2.29109500	-1.06762500	4.16332400
C	-3.28413300	1.18590200	4.20134700
C	-4.82928100	1.91780900	2.45949500
C	-1.60598800	-0.78489200	5.31487500
H	-2.14391300	-2.01875600	3.66951100
C	-2.56357500	1.43470800	5.41237400
C	-4.10613700	2.16222800	3.63125700
C	-1.75166400	0.47704200	5.95798700
H	-0.92561800	-1.52301800	5.72827800
H	-2.68136900	2.40419400	5.89171500
H	-4.20235200	3.12892100	4.12282600

H	-1.20716900	0.67795600	6.87673700
C	1.38942100	-2.26672300	-2.88302900
C	1.84600100	-1.02566700	-3.39325200
C	2.28984400	-3.13238700	-2.21378000
C	0.98150200	-0.08224200	-4.03972400
C	3.23916600	-0.66467200	-3.25593300
C	3.67033600	-2.73775000	-2.04766100
C	1.46076800	1.09720600	-4.54947900
H	-0.07484300	-0.31157400	-4.11328600
C	3.70319200	0.56890600	-3.81600000
C	4.11033500	-1.52285800	-2.57966700
C	2.84361000	1.42621900	-4.44951700
H	0.78016400	1.78919600	-5.03940600
H	4.76092800	0.80484400	-3.72598200
H	5.15242300	-1.23365100	-2.46111800
H	3.20971700	2.35648800	-4.87602000
C	-6.34843700	1.38263600	0.14479000
H	-6.94502900	1.18305600	-0.74107100
C	-5.53243000	0.40436400	0.65149400
H	-5.49213700	-0.56381000	0.16606200
C	-6.42966800	2.65868200	0.77209200
H	-7.09085500	3.41893400	0.36452600
C	-5.69007500	2.91379400	1.89716800
H	-5.76138100	3.87542800	2.40135000
C	2.79729300	-5.22182300	-1.05246900
H	2.47291500	-6.18634900	-0.67111800
C	4.14946300	-4.81604800	-0.86995100
H	4.84230900	-5.46935200	-0.34667200
C	4.57023300	-3.61005500	-1.35983600
H	5.60212200	-3.28983100	-1.23728700
C	1.90370700	-4.41279800	-1.70360000
H	0.88137000	-4.74549400	-1.83973900
C	-1.82056600	3.78010200	-0.77838600
C	-1.79183200	4.11636000	0.75687800
H	-1.50078100	5.16421200	0.89063000
H	-2.81995800	4.01810500	1.13726800
C	-0.94563600	3.25629500	1.62463300
C	-0.36468900	3.58253900	-1.26040100
H	0.21025300	4.49948800	-1.12921400
H	-0.36782800	3.32552000	-2.32550000
N	0.34823300	2.51090300	-0.55430400
C	1.63438300	2.59330000	-0.14284200
N	2.31723000	1.44414900	-0.00428900
C	3.68812000	1.35533800	0.40618700

C	4. 68184800	1. 68090300	-0. 51328800
C	4. 02087200	0. 87043800	1. 67166600
C	6. 02370400	1. 51499800	-0. 16887800
C	5. 36781900	0. 72499300	2. 00850300
H	3. 23962100	0. 58773700	2. 36846800
C	6. 37385100	1. 04004600	1. 09336400
H	7. 41539000	0. 90438200	1. 35770600
C	5. 73847100	0. 26428900	3. 39549100
C	7. 06869000	1. 78587600	-1. 21590600
F	6. 95288700	-0. 33068300	3. 41591800
F	4. 84384800	-0. 61057500	3. 89033300
F	5. 79740400	1. 30586400	4. 25912100
F	7. 02156800	0. 85410100	-2. 20806600
F	8. 31893800	1. 76628300	-0. 71517500
F	6. 88153400	2. 98313300	-1. 81193600
S	2. 29754600	4. 10445300	0. 38250300
H	4. 40242500	2. 03348100	-1. 49968500
H	1. 85688100	0. 54595100	-0. 18463400
H	0. 00563800	1. 55021200	-0. 75419100
C	0. 03711800	3. 79164200	2. 46410400
H	-0. 09461100	4. 85912600	2. 68025900
H	0. 95417400	3. 98171300	1. 57847800
N	-0. 57708900	-1. 23871900	1. 40688500
S	0. 92847100	-1. 36031300	1. 89527200
O	1. 17946400	-0. 51392900	3. 07489500
O	1. 93117900	-1. 30753700	0. 80460200
C	1. 03868600	-3. 10704700	2. 55232700
F	0. 76507900	-3. 98926900	1. 58845700
F	0. 16512600	-3. 28110800	3. 55749400
F	2. 27177200	-3. 33151000	3. 01522300
H	-1. 11227800	2. 18064300	1. 62434800
C	0. 66578600	2. 97173900	3. 58140100
H	0. 77935000	1. 91969900	3. 30262400
H	1. 65104200	3. 37014700	3. 84285000
H	0. 03645400	3. 00796600	4. 47732200
C	-2. 46634600	4. 98228600	-1. 49533400
C	-3. 75902500	5. 39276200	-1. 12392800
C	-1. 82506800	5. 70867300	-2. 50887600
C	-4. 37993700	6. 48151800	-1. 73281000
H	-4. 29931900	4. 85255900	-0. 35121800
C	-2. 44582500	6. 79948700	-3. 12384300
H	-0. 83082600	5. 43538400	-2. 84362400
C	-3. 72469700	7. 19380500	-2. 73891600
H	-5. 37933800	6. 77253700	-1. 41974100

H	-1.92019700	7.33865900	-3.90752000
H	-4.20652300	8.04293000	-3.21572100
C	-2.68381700	2.49865400	-1.02923300
H	-3.70605800	2.71293200	-0.70388100
H	-2.32301500	1.68649900	-0.38984400
C	-2.69606500	2.01088400	-2.45624800
H	-1.84978300	1.39630000	-2.76178500
C	-3.67563700	2.25101400	-3.33288400
H	-4.53296500	2.84726000	-3.01584000
C	-3.70460900	1.75633500	-4.75065500
H	-4.59228500	1.13683400	-4.93875900
H	-3.75027900	2.59145600	-5.46322700
H	-2.81902400	1.15599600	-4.98565600

TS-EF-4SS-2

l imaginary frequency

H = -5315.353121

G = -5315.554992

E(M06-2X-DCM) = -5316.233653

E(M06-2X-cyclohexane) = -5316.204590

O	-0.96460900	-1.92686700	-1.69299800
O	-2.89726400	-0.73448500	-0.41518000
P	-1.26477500	-0.85097000	-0.49114800
O	-0.74016600	0.51798400	-0.80276000
C	-2.08079900	-0.76333100	-5.55259200
C	-3.00905900	-1.32139900	-4.67890300
C	-2.60458800	-1.78932400	-3.42120600
C	-0.31895000	-1.06172300	-3.87387700
C	-0.74500600	-0.67603200	-5.15785000
C	-3.67065100	-1.87885300	-0.19783700
C	-3.92816000	-2.74539600	-1.26306500
C	-4.56331700	-3.97198000	-1.00670300
C	-5.02432200	-4.28585100	0.26635500
C	-4.87391200	-3.34846900	1.28678900
C	-4.19990700	-2.13345500	1.08435700
H	-0.00505000	-0.28272000	-5.84877300
H	-5.27598800	-3.55323300	2.27481500
C	-3.73223600	-2.57934100	-2.77048000
C	-4.96959400	-1.88971200	-3.43871000
H	-5.20166700	-0.97254700	-2.88511300
H	-5.86128400	-2.52426300	-3.42312900
H	-5.65922200	-4.82757600	-2.66945500
H	-4.35434200	-5.85573200	-2.08646300
C	-1.29418400	-1.58334900	-3.00083700

H	-2.38179300	-0.41247600	-6.53662000
H	-5.51241000	-5.23702100	0.46321700
C	-4.49650400	-1.53213400	-4.86679900
H	-4.99906400	-0.64408800	-5.26722100
H	-4.69684200	-2.35081400	-5.57211300
C	-4.63824000	-4.81186700	-2.26239400
C	-3.66545300	-4.08159900	-3.20969500
H	-2.64571300	-4.44826300	-3.04542900
H	-3.90249100	-4.21697100	-4.26956100
C	-4.18772500	-1.14264700	2.21104000
C	-3.37370200	-1.34383600	3.35014800
C	-5.13068000	-0.08441900	2.18999700
C	-2.44653500	-2.42846200	3.45250900
C	-3.47333100	-0.43500900	4.47127800
C	-5.23181200	0.80693200	3.32403900
C	-1.67124300	-2.59986900	4.56829800
H	-2.34140100	-3.10344200	2.61412700
C	-2.64540400	-0.64967200	5.61833300
C	-4.39053600	0.61772200	4.42394000
C	-1.77016600	-1.70123100	5.66824700
H	-0.95548900	-3.41510400	4.60256000
H	-2.73799400	0.03824100	6.45612700
H	-4.47409900	1.28854700	5.27725700
H	-1.14613900	-1.85456900	6.54469100
C	1.12737300	-0.95023300	-3.50709800
C	1.76767500	0.31526200	-3.51222400
C	1.88065500	-2.12110100	-3.23550800
C	1.07251500	1.54156600	-3.77367000
C	3.18753800	0.40175000	-3.24739600
C	3.28922400	-2.01234800	-2.92990900
C	1.73481300	2.74226500	-3.83158500
H	0.00088700	1.50913500	-3.93128000
C	3.83778100	1.67595100	-3.30501700
C	3.90546600	-0.75872400	-2.94735600
C	3.13888500	2.81593500	-3.59955400
H	1.18425800	3.65047600	-4.06645000
H	4.90978000	1.71104600	-3.12210400
H	4.96815000	-0.68261800	-2.72599900
H	3.64709100	3.77476000	-3.65651400
C	-6.99614000	1.10644300	1.14660400
H	-7.69082300	1.22193400	0.31876700
C	-6.04841900	0.11655000	1.10757500
H	-6.00066500	-0.54761600	0.25201100
C	-7.08822700	1.98246800	2.26598700

H	-7.85062300	2.75672500	2.28323300
C	-6.22217400	1.83883200	3.31632800
H	-6.28538800	2.49600300	4.18086000
C	2.06903400	-4.54608300	-2.99503500
H	1.60986100	-5.53036500	-3.02814100
C	3.44785900	-4.42818800	-2.66271000
H	4.02645900	-5.31976900	-2.43729600
C	4.03807800	-3.19456100	-2.63809100
H	5.09328200	-3.08762200	-2.39876200
C	1.31654900	-3.43590500	-3.27431700
H	0.27147000	-3.55165700	-3.53528200
C	-0.71197100	4.43507700	-0.05285700
C	-0.92977200	4.33372800	1.48692100
H	-0.37302600	5.12336600	2.00176100
H	-2.00129200	4.50770800	1.67879700
C	-0.57488100	3.03056800	2.11325900
C	0.70424700	3.89430400	-0.38708800
H	1.45801500	4.55846700	0.03619100
H	0.84425500	3.87017800	-1.47148500
N	0.98787100	2.53497600	0.10016400
C	2.16010300	2.19126100	0.68261200
N	2.60289500	0.93376100	0.54175200
C	3.88558500	0.47695200	0.98890300
C	5.01069200	0.87972100	0.27279600
C	4.00065000	-0.42323300	2.04814100
C	6.26656800	0.38124100	0.61702600
C	5.26682100	-0.90134300	2.39269100
H	3.11443700	-0.75811900	2.57687700
C	6.40223600	-0.50673600	1.68258600
H	7.37738700	-0.89328100	1.95235000
C	5.39745400	-1.90938100	3.50703500
C	7.45554300	0.81849900	-0.19440100
F	6.63331600	-1.88314800	4.05785000
F	5.18910800	-3.16818900	3.06529600
F	4.50743100	-1.67945000	4.49327600
F	7.20214400	0.70833900	-1.52614700
F	8.55435300	0.08446200	0.06807300
F	7.76971200	2.11329200	0.02810100
S	2.94183300	3.30033200	1.76475600
H	4.89437800	1.55758200	-0.56549200
H	2.03875100	0.21697800	0.06590400
H	0.46383600	1.77494400	-0.36858400
C	0.25426800	2.95563400	3.23231300
H	0.32218000	3.88592000	3.80939600

H	1.40076400	3.17281000	2.61565900
N	-0.82657800	-1.60459000	0.86845100
S	0.65884100	-2.05029000	1.17522800
O	1.03002600	-1.78694200	2.57628100
O	1.64846700	-1.65691600	0.13725500
C	0.60413600	-3.91551600	1.05597900
F	0.18805200	-4.29913200	-0.15308700
F	-0.23421400	-4.41536700	1.97857700
F	1.82506300	-4.41105200	1.27733400
H	-0.98386900	2.11471100	1.69077100
C	0.41048000	1.67227400	4.03300100
H	0.42168200	0.78475100	3.39262200
H	1.34276900	1.68744300	4.60589900
H	-0.41729300	1.55552300	4.74131200
C	-0.74749100	5.90512700	-0.52582800
C	-1.11451600	6.97400800	0.30463600
C	-0.42768100	6.20844300	-1.86188400
C	-1.14200800	8.28793900	-0.16975500
H	-1.39989900	6.79966500	1.33584200
C	-0.44991400	7.51816400	-2.33824500
H	-0.16696800	5.41241700	-2.55301800
C	-0.80411500	8.56915700	-1.49145000
H	-1.43279800	9.09070800	0.50263900
H	-0.19292300	7.71475700	-3.37574900
H	-0.82279500	9.59100500	-1.85988100
C	-1.81525100	3.62658500	-0.81406700
H	-1.83525300	2.58780000	-0.47010200
H	-1.51058600	3.57697600	-1.86943700
C	-3.18799900	4.23634800	-0.72887200
H	-3.28862200	5.24593600	-1.12844300
C	-4.27585500	3.63622700	-0.23525600
H	-4.20105200	2.62001400	0.15463700
C	-5.64022000	4.26316900	-0.20241200
H	-6.36086600	3.66792700	-0.77886500
H	-6.02963800	4.31003600	0.82219500
H	-5.62658000	5.27752800	-0.61623600

TS-EF-4SS-3

l imaginary frequency

H = -5315.353020

G = -5315.555409

E(M06-2X-DCM) = -5316.234197

E(M06-2X-cyclohexane) = -5316.208055

O	1.08482600	-2.63688400	0.71322400
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O	3.08324300	-1.04130000	0.28956900
P	1.44858100	-1.09977500	0.27881500
O	0.94751900	-0.06758200	1.24079600
C	2.26775700	-3.84566600	4.54095000
C	3.14689100	-3.92454600	3.46534500
C	2.72086600	-3.58808800	2.17256100
C	0.51829800	-3.00227800	3.04863300
C	0.95918100	-3.41571400	4.31793100
C	3.81146700	-1.89323300	-0.54533400
C	4.00766300	-3.22455300	-0.17530700
C	4.58253300	-4.11007000	-1.10208100
C	5.05759200	-3.65296000	-2.32610100
C	4.97281400	-2.29193400	-2.61847500
C	4.34656700	-1.38696600	-1.74698100
H	0.25738700	-3.37198600	5.14571700
H	5.38329000	-1.91068100	-3.54901500
C	3.79562100	-3.94775200	1.15465700
C	5.07157500	-3.84998000	2.05968700
H	5.38130000	-2.80006000	2.11753000
H	5.91289600	-4.42474900	1.66016500
H	5.58160900	-5.84098700	-0.25933800
H	4.23021200	-6.25234300	-1.30962100
C	1.44059800	-3.07456700	1.98735300
H	2.58883100	-4.11650900	5.54367000
H	5.50366700	-4.33932600	-3.04139700
C	4.60453200	-4.33131500	3.45159600
H	5.17600400	-3.87738600	4.26928600
H	4.71546400	-5.41979600	3.55652700
C	4.57438200	-5.52504000	-0.56547400
C	3.62447000	-5.41829500	0.64622900
H	2.58819200	-5.55724700	0.31760100
H	3.82963300	-6.15660600	1.42774700
C	4.35301400	0.07103700	-2.09366400
C	3.58350700	0.55997000	-3.17636800
C	5.23736200	0.93665700	-1.40152000
C	2.68605200	-0.26884600	-3.92265500
C	3.68643000	1.95181100	-3.55721000
C	5.33910800	2.32287100	-1.79997100
C	1.95082500	0.23334800	-4.96336100
H	2.56737100	-1.30348800	-3.62969200
C	2.90353500	2.43522800	-4.65303300
C	4.55578900	2.79385200	-2.85829000
C	2.06207100	1.60219000	-5.33980000
H	1.25766700	-0.41433400	-5.49135300

H	2.99984900	3.48242300	-4.93161700
H	4.64419100	3.83591600	-3.16093400
H	1.47272900	1.98063500	-6.17083100
C	-0.88764000	-2.52335700	2.87234600
C	-1.32036400	-1.35196900	3.54356500
C	-1.79890700	-3.26697000	2.08227000
C	-0.43798000	-0.52214500	4.30990300
C	-2.70392500	-0.94304100	3.44836900
C	-3.16806300	-2.82006500	1.95967600
C	-0.89437200	0.59077100	4.96903300
H	0.61354400	-0.77866400	4.35164300
C	-3.14041700	0.22237200	4.15468100
C	-3.58694800	-1.68444400	2.65818800
C	-2.26734600	0.96624900	4.90189100
H	-0.20144100	1.19575500	5.54839700
H	-4.18893900	0.50280300	4.08380300
H	-4.62480500	-1.36662600	2.58019700
H	-2.61392800	1.84525200	5.43906900
C	6.96120800	1.34209700	0.28640100
H	7.59544600	0.97330900	1.08794600
C	6.08508800	0.49170600	-0.33565100
H	6.03622400	-0.54638200	-0.02788000
C	7.05734000	2.70579700	-0.11156000
H	7.76659700	3.36310400	0.38417900
C	6.26480000	3.17867100	-1.12341200
H	6.33513500	4.21554600	-1.44459300
C	-2.32810400	-5.13637300	0.59958300
H	-2.01711900	-6.03740800	0.07776600
C	-3.66318300	-4.66546700	0.44828400
H	-4.35535900	-5.19404100	-0.20093000
C	-4.07094100	-3.54648000	1.12154900
H	-5.08888400	-3.18128500	1.01697900
C	-1.43280900	-4.46585600	1.39083000
H	-0.42261400	-4.84400100	1.49585200
C	0.90574800	3.61058800	1.17347800
C	1.28754200	2.98743200	-0.20072800
H	2.16452300	3.50950700	-0.60841200
H	1.61604000	1.96427400	-0.00866600
C	0.24823400	2.93631400	-1.27643900
C	-0.40271300	2.91052300	1.71314000
H	-1.15825900	3.65469700	1.95168600
H	-0.15796200	2.35911000	2.62530100
N	-1.05170500	1.92131800	0.83673400
C	-2.33531900	2.01758800	0.42016800

N	-2.97410500	0.86428900	0.13819900
C	-4.29081400	0.63384500	-0.32807900
C	-5.38400900	1.43706500	0.01540200
C	-4.49650400	-0.52463400	-1.09260900
C	-6.65884700	1.09920300	-0.44176800
C	-5.77928100	-0.85605100	-1.51949900
H	-3.65424100	-1.15952000	-1.34185000
C	-6.87049600	-0.04328800	-1.21124000
H	-7.86354100	-0.29386200	-1.56449600
C	-5.99603200	-2.14762200	-2.26546100
C	-7.83585700	1.94264900	-0.02325500
F	-4.91230300	-2.51382300	-2.97529700
F	-7.04027600	-2.06322500	-3.11809900
F	-6.27344900	-3.16593900	-1.40996900
F	-8.35992500	1.51189800	1.14849300
F	-8.82930300	1.90319900	-0.93676600
F	-7.49184600	3.23611600	0.15284700
S	-2.99749500	3.58824500	0.11888700
H	-5.25561900	2.31565100	0.63157100
H	-2.38152600	0.02253800	0.09925900
H	-0.60724700	0.99196300	0.90428000
C	-0.58414400	3.95776300	-1.72229000
H	-0.32693400	4.97428100	-1.41640000
H	-1.57567200	3.81696700	-0.84757000
N	1.02769900	-1.00402300	-1.28597700
S	-0.46584200	-1.07748300	-1.77586600
O	-0.80226600	-0.01188200	-2.73521900
O	-1.45624600	-1.32138300	-0.68476500
C	-0.55777500	-2.65499400	-2.77001900
F	0.26464100	-2.59253900	-3.82762300
F	-1.81098500	-2.82009600	-3.20927900
F	-0.21488400	-3.70108900	-2.01733000
C	0.76161900	5.14514000	1.16639200
C	0.10912700	5.79690800	2.22714500
C	1.36556000	5.95917600	0.19589100
C	0.02887800	7.18762700	2.29551500
H	-0.33971100	5.21861000	3.02981500
C	1.28567500	7.35239300	0.25559700
H	1.91438400	5.51407300	-0.62733000
C	0.61152600	7.97620000	1.30358300
H	-0.49114200	7.65271500	3.12884900
H	1.75904800	7.94746300	-0.52109700
H	0.54688100	9.05966600	1.35110400
C	2.04848800	3.24668800	2.19867300

H	1.71790600	3.59067500	3.18691200
H	2.10015300	2.15033100	2.23824200
C	3.40951500	3.81708500	1.91271700
C	3.98448400	4.78102500	2.63905900
H	3.43365200	5.19573000	3.48577000
H	3.95899500	3.39192200	1.07198300
H	0.14644700	1.97471300	-1.78244000
C	-1.29045400	3.82328800	-3.06704700
H	-1.53406000	2.77734600	-3.27733200
H	-2.21564000	4.40785200	-3.08692400
H	-0.64272300	4.18863800	-3.87224800
C	5.34676000	5.36193000	2.39416900
H	5.28649500	6.44181600	2.20027000
H	5.99561900	5.23823900	3.27219600
H	5.83666900	4.88583800	1.53920700

TS-EF-4SS-4

l imaginary frequency

H = -5315.351455

G = -5315.552355

E(M06-2X-DCM) = -5316.233776

E(M06-2X-cyclohexane) = -5316.207887

O	0.94801300	-2.70939300	0.58243900
O	2.97728800	-1.09318400	0.54850600
P	1.36623300	-1.15740800	0.27022400
O	0.72469900	-0.17324200	1.19950200
C	1.41585000	-3.92047600	4.56346800
C	2.48308900	-3.97523500	3.67285000
C	2.30045700	-3.64544300	2.32202600
C	-0.04368400	-3.12395200	2.76450000
C	0.16168600	-3.52810300	4.09541800
C	3.84960800	-1.93148200	-0.14810200
C	3.99991900	-3.25857300	0.25714200
C	4.75393800	-4.13391900	-0.54112900
C	5.43912600	-3.66851300	-1.65784400
C	5.37705900	-2.31168300	-1.97152800
C	4.58034300	-1.41700100	-1.23762200
H	-0.68555900	-3.50818100	4.77452700
H	5.94056700	-1.92511400	-2.81558800
C	3.55638600	-3.98222300	1.52774700
C	4.63646400	-3.85516200	2.65595900
H	4.90633100	-2.79844300	2.76659600
H	5.55064400	-4.41049100	2.42417600
H	5.61493600	-5.83968000	0.48448900

H	4. 49240700	-6. 28398800	-0. 79659600
C	1. 06528700	-3. 16252500	1. 89815300
H	1. 54931200	-4. 18402300	5. 60971800
H	6. 02658800	-4. 34555800	-2. 27282000
C	3. 92617800	-4. 34691100	3. 93660300
H	4. 32179800	-3. 87898800	4. 84536600
H	4. 04112600	-5. 43228200	4. 06629600
C	4. 67595300	-5. 54719700	-0. 00626100
C	3. 51469200	-5. 45790100	1. 00624400
H	2. 56107800	-5. 62124900	0. 49134100
H	3. 58601400	-6. 18920600	1. 81737700
C	4. 60704000	0. 03268200	-1. 61438900
C	4. 09840800	0. 45018300	-2. 86874100
C	5. 26183900	0. 96388800	-0. 76843700
C	3. 39437500	-0. 43297300	-3. 74843800
C	4. 27036400	1. 82228500	-3. 29236800
C	5. 41620500	2. 33587100	-1. 19954800
C	2. 91527000	-0. 00206600	-4. 95702200
H	3. 20654500	-1. 44868000	-3. 42652500
C	3. 76739600	2. 22768200	-4. 56876300
C	4. 92448200	2. 72520100	-2. 44948900
C	3. 11257900	1. 34252900	-5. 38145900
H	2. 35806400	-0. 68775300	-5. 58817700
H	3. 91702100	3. 26023400	-4. 87649100
H	5. 06382200	3. 75374600	-2. 77803600
H	2. 73009900	1. 66329600	-6. 34675500
C	-1. 41376300	-2. 71075900	2. 32889500
C	-2. 02851400	-1. 57682700	2. 91673700
C	-2. 12784700	-3. 50170400	1. 39428200
C	-1. 33936000	-0. 69469900	3. 81217100
C	-3. 40497000	-1. 26514600	2. 60144400
C	-3. 48315700	-3. 14243600	1. 04376500
C	-1. 97274000	0. 37699700	4. 38705500
H	-0. 29073300	-0. 87448700	4. 01588600
C	-4. 03518800	-0. 14748800	3. 23678700
C	-4. 09085200	-2. 05180800	1. 67216800
C	-3. 34348600	0. 64949600	4. 10933100
H	-1. 42372900	1. 02906700	5. 06157900
H	-5. 07714700	0. 05918200	3. 00307500
H	-5. 12262400	-1. 80736300	1. 42870800
H	-3. 83264500	1. 49412300	4. 58760200
C	6. 45359300	1. 52731900	1. 29353700
H	6. 86540800	1. 22343100	2. 25213500
C	5. 81892500	0. 60552300	0. 50169400

H	5.73840200	-0.42210800	0.83641300
C	6.58991600	2.87980200	0.86970800
H	7.10106300	3.59618700	1.50709200
C	6.08928400	3.26617000	-0.34511600
H	6.20551400	4.29077100	-0.69221500
C	-2.28638800	-5.39701500	-0.14051500
H	-1.83840400	-6.27676100	-0.59482500
C	-3.60472600	-5.01098400	-0.51367000
H	-4.14549600	-5.58860900	-1.25833100
C	-4.18605900	-3.91807700	0.06921000
H	-5.18796200	-3.60635600	-0.21307700
C	-1.57672800	-4.67141500	0.77988300
H	-0.57587700	-4.98551000	1.05187500
C	1.30328100	3.52138100	0.83163500
C	1.47058000	2.92386300	-0.61118300
H	2.35696700	3.39078200	-1.06634600
H	1.70587000	1.86097300	-0.52326200
C	0.35583500	3.06024100	-1.59388200
C	-0.06545700	3.04633500	1.44639800
H	-0.74111700	3.87294000	1.63984100
H	0.13971600	2.56037200	2.40330200
N	-0.81396400	2.05840800	0.65566400
C	-2.09096800	2.19398100	0.25577200
N	-2.73203900	1.06415500	-0.11328100
C	-4.09790500	0.90239200	-0.44161600
C	-4.43422000	-0.01509800	-1.44674500
C	-5.10610600	1.54387800	0.28054400
C	-5.77557000	-0.26401000	-1.72849000
C	-6.44411800	1.28283300	-0.01666500
H	-4.85540900	2.21615300	1.09087400
C	-6.79156800	0.38525000	-1.02293200
H	-7.83261700	0.18977100	-1.25026900
C	-7.50117300	1.91539000	0.84849500
C	-6.15321900	-1.29463100	-2.76062500
F	-7.54755500	1.31959300	2.06794000
F	-8.73261700	1.81440200	0.30959300
F	-7.25355000	3.22417200	1.06774400
F	-7.22777100	-0.90248800	-3.48075900
F	-6.49063800	-2.47321200	-2.17694000
F	-5.15134300	-1.54889700	-3.62182400
S	-2.77497600	3.77487800	0.04084500
H	-3.64871500	-0.53585800	-1.98260100
H	-2.15723300	0.22305000	-0.26671500
H	-0.42422100	1.10165100	0.75617600

C	-0.40554600	4.19089700	-1.88238300
H	-0.02940900	5.14209700	-1.50038100
H	-1.36279200	4.01985600	-1.00085100
N	1.20443900	-0.97808900	-1.33098900
S	-0.17658700	-0.97252300	-2.09352400
O	-0.24604500	0.09923400	-3.10092900
O	-1.37310200	-1.13633600	-1.21803800
C	-0.15601700	-2.55777400	-3.08195300
F	0.87558200	-2.56118200	-3.93918500
F	-1.29214700	-2.65814900	-3.77878600
F	-0.04407800	-3.60861100	-2.26834000
C	1.47186000	5.06212800	0.77933600
C	0.43041100	5.98389800	0.96956700
C	2.74450000	5.58887400	0.49164700
C	0.64969700	7.36239800	0.88259500
H	-0.58131700	5.65127100	1.17295400
C	2.96711300	6.96142200	0.40301800
H	3.58593400	4.91967300	0.34046500
C	1.91867600	7.86121400	0.60031600
H	-0.18397700	8.04245600	1.03711700
H	3.96667900	7.32745600	0.18285200
H	2.08960200	8.93213000	0.53442900
C	2.44411900	2.86035200	1.66921000
H	2.26684900	1.77646100	1.64283700
H	3.40434900	2.99589300	1.15496800
C	2.63014700	3.25230200	3.11464900
C	1.98117000	4.15647800	3.85433900
H	1.19551100	4.76444700	3.40968300
H	3.41935500	2.67516000	3.60200600
H	0.13163700	2.15617600	-2.16596300
C	-1.18261500	4.26791100	-3.19376200
H	-1.52704700	3.27707200	-3.50590400
H	-2.05505700	4.92138300	-3.09595800
H	-0.54497900	4.67267000	-3.98770900
C	2.27074900	4.43012900	5.30409100
H	2.56827400	5.47618300	5.45952200
H	1.38278100	4.26216000	5.92893200
H	3.07508600	3.78946100	5.68184200

TS-EF-4SR

l imaginary frequency

H = -5315.352154

G = -5315.553120

E(M06-2X-DCM) = -5316.241096

E(M06-2X-cyclohexane) = -5316.210985

O	-0.68455000	-2.46233800	-0.85770200
O	-2.62723900	-0.94812200	-0.04076200
P	-0.98932300	-1.03963000	-0.09659900
O	-0.50120300	0.14203000	-0.87617600
C	-1.93022800	-2.75365000	-4.84162400
C	-2.81061200	-3.02133600	-3.79800400
C	-2.36501000	-2.99881300	-2.46890200
C	-0.13392200	-2.35584900	-3.22304300
C	-0.59905000	-2.45822300	-4.54615400
C	-3.36322900	-1.94904300	0.59452000
C	-3.62234400	-3.14553300	-0.07778600
C	-4.22302400	-4.20543000	0.62174500
C	-4.66249700	-4.03969000	1.93000300
C	-4.50668500	-2.79674800	2.54137000
C	-3.85100500	-1.73299800	1.90050700
H	0.10522000	-2.28082000	-5.35369400
H	-4.87951200	-2.63844300	3.54910300
C	-3.44907200	-3.54006400	-1.54496600
C	-4.72445400	-3.18741700	-2.38366400
H	-4.98939600	-2.14034600	-2.19540400
H	-5.58772400	-3.80333500	-2.11305300
H	-5.30162900	-5.64337600	-0.59274900
H	-3.96304700	-6.34749400	0.30803500
C	-1.06008100	-2.60055700	-2.19021700
H	-2.26528700	-2.78415000	-5.87557300
H	-5.12991500	-4.86009500	2.46867600
C	-4.28560700	-3.35700100	-3.85540900
H	-4.84088000	-2.70535300	-4.54039700
H	-4.44712900	-4.38662400	-4.20435300
C	-4.27995700	-5.45042700	-0.23600600
C	-3.33363400	-5.09505300	-1.40131400
H	-2.30189400	-5.34540700	-1.12946900
H	-3.57093200	-5.61936500	-2.33230300
C	-3.76206700	-0.41846700	2.61362100
C	-2.97266800	-0.29079600	3.78211200
C	-4.57103400	0.66286300	2.18329900
C	-2.12899100	-1.34258700	4.26210200
C	-2.99704000	0.94584800	4.53172900
C	-4.55129600	1.90932000	2.91633600
C	-1.38930400	-1.19604100	5.40516900
H	-2.04949800	-2.25267800	3.68279700
C	-2.22287200	1.05089500	5.73037300
C	-3.77085900	2.01475500	4.07116800

C	-1.44434900	0.01024800	6.15906800
H	-0.73349600	-1.99965500	5.72569300
H	-2.26747900	1.98114900	6.29265600
H	-3.78110900	2.94566700	4.63556600
H	-0.85459400	0.10406200	7.06689600
C	1.30571100	-2.03406500	-2.97292500
C	1.84244000	-0.80048600	-3.42012400
C	2.15391800	-2.99738000	-2.37048700
C	1.03877900	0.23438600	-4.00258700
C	3.25963300	-0.54501500	-3.28546100
C	3.55854400	-2.70454100	-2.19600900
C	1.59915500	1.39552500	-4.47173400
H	-0.03418500	0.09425700	-4.05912600
C	3.80497400	0.67704800	-3.79488800
C	4.07535500	-1.49364600	-2.66357700
C	3.00334600	1.61994700	-4.38127500
H	0.96432600	2.15363400	-4.92398000
H	4.87745100	0.83412500	-3.70542400
H	5.13479300	-1.28071000	-2.53789800
H	3.43125700	2.53839500	-4.77462900
C	-6.23295500	1.63398000	0.67048500
H	-6.90423500	1.53062600	-0.17790700
C	-5.45981500	0.57140100	1.06329200
H	-5.52770300	-0.37017700	0.52965700
C	-6.17323400	2.87395500	1.36876600
H	-6.78914600	3.70736300	1.04167100
C	-5.35835000	3.00035200	2.46213700
H	-5.32324600	3.93242100	3.02213400
C	2.53455500	-5.18466900	-1.34901800
H	2.15128600	-6.14899100	-1.02648100
C	3.91038900	-4.87751300	-1.15274000
H	4.56262600	-5.60468800	-0.67692100
C	4.40465000	-3.67251400	-1.57086100
H	5.45546900	-3.42640300	-1.43879600
C	1.69065100	-4.28103400	-1.93899700
H	0.64899300	-4.54023800	-2.08626600
C	-1.44983700	4.09363700	-1.51766100
C	-1.75384100	4.25796600	0.00609800
H	-1.48853000	5.28190000	0.29318600
H	-2.83891300	4.17901700	0.16317500
C	-1.08105200	3.31660000	0.94607800
C	0.07264300	3.86179400	-1.68822900
H	0.62532500	4.73378100	-1.33690200
H	0.30911100	3.71924700	-2.74813900

N	0.57944500	2.69548100	-0.95829900
C	1.75534000	2.66598400	-0.29604600
N	2.33120500	1.47576800	-0.06309200
C	3.66472000	1.32834500	0.44981800
C	4.72662100	1.58084500	-0.41500000
C	3.89807300	0.87422200	1.74802300
C	6.03713700	1.37022000	0.01525500
C	5.21490700	0.68372700	2.17059200
H	3.06695700	0.64301600	2.40486400
C	6.28838400	0.92411700	1.31056700
H	7.30446500	0.75192000	1.64338700
C	5.47825500	0.25102900	3.59119400
C	7.15173300	1.58095200	-0.97174600
F	6.67963900	-0.35974300	3.71207600
F	4.53822600	-0.59829600	4.04057200
F	5.49241400	1.31315600	4.43193700
F	7.06317600	0.70220400	-2.00817900
F	8.36955500	1.42134900	-0.41941300
F	7.10736800	2.81545500	-1.51968000
S	2.37285300	4.11518700	0.43565400
H	4.52354800	1.91206900	-1.42741000
H	1.84537300	0.60998500	-0.31911100
H	0.16960800	1.77774800	-1.19681900
C	-0.27003800	3.77061800	1.98773700
H	-0.42360800	4.82442100	2.25092700
H	0.82817900	4.00382500	1.30185500
N	-0.53269800	-1.26125700	1.43411400
S	0.98718100	-1.42383800	1.85943400
O	1.28437000	-0.66859400	3.08849900
O	1.95356700	-1.30446600	0.74154500
C	1.10041500	-3.21531500	2.38150700
F	0.77583700	-4.02172700	1.36706700
F	0.26818800	-3.45986800	3.40720000
F	2.34920600	-3.48732200	2.77349600
C	-2.24877500	2.98588900	-2.23067400
C	-3.19962900	2.18106600	-1.59530800
C	-2.05111500	2.79083500	-3.61124900
C	-3.92493900	1.22189500	-2.30753100
H	-3.39330400	2.27215900	-0.53284400
C	-2.77205300	1.83675900	-4.32442900
H	-1.33081000	3.39963100	-4.15101200
C	-3.71806300	1.04427100	-3.67167700
H	-4.64693300	0.61246300	-1.77513800
H	-2.59656300	1.71660900	-5.39026700

H	-4.28070900	0.29586400	-4.22252200
C	-1.77324700	5.47180500	-2.19406800
H	-1.12970200	6.24134400	-1.74786200
H	-1.49027600	5.40593000	-3.25316800
C	-3.21259900	5.89582300	-2.08936000
C	-3.63134900	7.02514100	-1.50964100
H	-2.89113600	7.69803400	-1.07110100
H	-3.94620900	5.22288500	-2.53392300
H	-1.23762900	2.24716500	0.81708100
C	-5.06219900	7.47206500	-1.41850200
H	-5.20883300	8.43741400	-1.92146500
H	-5.74110200	6.74486800	-1.87611500
H	-5.36891100	7.61480300	-0.37350500
C	0.15131600	2.86660300	3.13675100
H	0.31343900	1.83344200	2.81559600
H	1.07705100	3.23026000	3.59327900
H	-0.62364800	2.84981700	3.90989800

TS-EF-4SR-1

l imaginary frequency

H = -5315.352799

G = -5315.555698

E(M06-2X-DCM) = -5316.235969

E(M06-2X-cyclohexane) = -5316.209472

O	-1.53236000	-2.61116500	-0.20373600
O	-3.04920600	-0.53421900	0.11499000
P	-1.48408800	-0.98473200	-0.01907000
O	-0.93886700	-0.26965200	-1.21772900
C	-3.31452700	-3.93861200	-3.74997300
C	-4.08786000	-3.65642000	-2.62828800
C	-3.48024900	-3.29160100	-1.41778600
C	-1.28606000	-3.41197500	-2.48419000
C	-1.92486000	-3.84517200	-3.65842800
C	-3.86337200	-1.07594900	1.11180100
C	-4.42458100	-2.34068300	0.92963400
C	-5.11575600	-2.93750800	1.99658600
C	-5.33988000	-2.24117100	3.17909000
C	-4.87299800	-0.93237900	3.29284800
C	-4.11877400	-0.32411400	2.27578700
H	-1.30958200	-4.08734200	-4.52012500
H	-5.07338500	-0.36273700	4.19547400
C	-4.52045600	-3.23706200	-0.30511500
C	-5.80226700	-2.91295700	-1.14592500
H	-5.83897200	-1.83262000	-1.32860200

H	-6.72439500	-3.19486000	-0.62827900
H	-6.59648200	-4.42216800	1.44163400
H	-5.30876300	-5.06044200	2.45814700
C	-2.10078000	-3.11114800	-1.37611700
H	-3.78009300	-4.23227500	-4.68751500
H	-5.87993200	-2.70219900	4.00222600
C	-5.59448000	-3.66049000	-2.48227500
H	-6.10017600	-3.17195900	-3.32311000
H	-5.98758600	-4.68562700	-2.43224700
C	-5.51895400	-4.35350300	1.64747500
C	-4.68421100	-4.63522700	0.38046900
H	-3.69236400	-5.00436600	0.66532800
H	-5.13804200	-5.37591000	-0.28536500
C	-3.67694300	1.09546500	2.45628600
C	-2.75440400	1.42760300	3.47865400
C	-4.26809200	2.11869800	1.67232900
C	-2.09181600	0.43902300	4.27485100
C	-2.43635300	2.81515300	3.73319100
C	-3.92463800	3.50070300	1.92471300
C	-1.20741700	0.79178000	5.25947400
H	-2.26930400	-0.60704600	4.06188800
C	-1.51949400	3.14128300	4.78219400
C	-3.02740700	3.81063500	2.95080600
C	-0.92436100	2.16089600	5.52876600
H	-0.69892100	0.01778100	5.82660500
H	-1.30708600	4.19133900	4.97141300
H	-2.78714600	4.85386800	3.14823100
H	-0.22537200	2.42029900	6.31933100
C	0.20557500	-3.30496000	-2.44013700
C	0.87303700	-2.36220700	-3.26038400
C	0.95123100	-4.18810800	-1.62060900
C	0.17943700	-1.42636600	-4.09564100
C	2.31835000	-2.31338900	-3.26235000
C	2.39405500	-4.11118200	-1.61513200
C	0.85680800	-0.54480700	-4.89869800
H	-0.90344000	-1.41343400	-4.07611700
C	2.98643300	-1.37500300	-4.11184600
C	3.03698500	-3.18191800	-2.43676400
C	2.28160800	-0.51943400	-4.91496100
H	0.30181300	0.14538000	-5.52909600
H	4.07425500	-1.36479700	-4.10925600
H	4.12441900	-3.13811800	-2.43816300
H	2.80163500	0.18110400	-5.56311900
C	-5.77262800	2.86781200	-0.10540400

H	-6.49063900	2.63549700	-0.88704600
C	-5.22506500	1.85604300	0.63934500
H	-5.52104700	0.83093900	0.44893500
C	-5.41438800	4.22451600	0.13441100
H	-5.85923500	5.01335400	-0.46601800
C	-4.52137400	4.52749800	1.12656300
H	-4.25068400	5.56064700	1.33361300
C	1.09060300	-6.02280800	-0.01208000
H	0.59819800	-6.76973200	0.60486000
C	2.51085300	-5.92749900	0.00443900
H	3.08866300	-6.59582400	0.63697300
C	3.14009000	-4.99986200	-0.77992900
H	4.22457000	-4.91996700	-0.78402700
C	0.34055900	-5.18753200	-0.79754900
H	-0.73902800	-5.28359200	-0.80290600
C	-0.62042100	3.48889100	-2.00028800
C	-1.05087400	3.19068700	-0.51880900
H	-1.68329500	4.02761200	-0.19514300
H	-1.67787200	2.29995200	-0.50657900
C	0.03016200	2.99992500	0.50244600
C	0.44352000	2.42978900	-2.49575600
H	1.22842200	2.94396800	-3.05307900
H	-0.03983200	1.72135600	-3.16899900
N	1.09026700	1.58363800	-1.47827800
C	2.37865500	1.64216800	-1.10317800
N	2.93527300	0.53833100	-0.57107800
C	4.25899500	0.44636300	-0.04761500
C	5.35760100	0.64267200	-0.88724700
C	4.44411200	0.08980100	1.28994800
C	6.64772900	0.50468700	-0.37818300
C	5.74336700	-0.06010500	1.78057700
H	3.58440400	-0.05093100	1.93723200
C	6.84794000	0.14982800	0.95642700
H	7.85190600	0.03530500	1.34722300
C	5.94925600	-0.50291300	3.20757700
C	7.83233000	0.78241000	-1.26634200
F	5.91336500	-1.84971400	3.31600400
F	4.99738100	-0.01179000	4.02529900
F	7.14845700	-0.10004600	3.68560500
F	7.56529200	0.49293600	-2.55958500
F	8.91229600	0.05882100	-0.90068300
F	8.19445700	2.08396900	-1.22043500
S	3.20453300	3.17135000	-1.11496200
H	5.20340700	0.88646200	-1.93180200

H	2.33171400	-0.27285000	-0.36288700
H	0.55677100	0.71177700	-1.30960400
C	0.99838300	3.91546200	0.88704200
H	0.83323300	4.95110500	0.57952100
H	1.94218000	3.63272800	-0.07044200
N	-0.82996500	-0.73341100	1.44013800
S	0.67444500	-1.05954100	1.79190100
O	1.28552600	0.00219300	2.61119300
O	1.49228800	-1.55167900	0.64710900
C	0.56832300	-2.53977100	2.92913500
F	-0.00901700	-3.56587900	2.30230000
F	-0.15012600	-2.23657600	4.01963200
F	1.79986100	-2.89162100	3.31056300
C	-1.87449200	3.34892700	-2.90371600
C	-2.59163600	2.13738400	-2.90589100
C	-2.31857000	4.36315600	-3.76493900
C	-3.70919400	1.95984000	-3.71902000
H	-2.26868500	1.30827800	-2.28270900
C	-3.43966400	4.18569200	-4.58148100
H	-1.80018000	5.31297700	-3.81995300
C	-4.14406300	2.98507400	-4.56095400
H	-4.23710900	1.01014100	-3.69403600
H	-3.75446300	4.99474100	-5.23570800
H	-5.01515000	2.84634000	-5.19592500
C	0.01617300	4.90596800	-2.12528800
H	1.02412300	4.88581400	-1.70499000
H	0.16857000	5.09666600	-3.19743300
C	-0.75734900	6.04687700	-1.50941600
C	-0.19957300	7.07448900	-0.85918600
H	0.88660800	7.09880700	-0.74354300
H	-1.84085200	6.03630200	-1.62934500
H	0.02980900	2.04147900	1.02230600
C	1.77001700	3.71950400	2.18583200
H	1.87820600	2.65678300	2.42338200
H	2.76625300	4.17002700	2.12854000
H	1.23243300	4.19186300	3.01605200
C	-0.94767000	8.24157500	-0.28068000
H	-0.76025600	8.34220900	0.79680900
H	-0.62776200	9.18554100	-0.74229300
H	-2.02795000	8.14111700	-0.43038800

TS-EF-4SR-2

l imaginary frequency

H = -5315.350501

G = -5315.553732

E(M06-2X-DCM) = -5316.233008

E(M06-2X-cyclohexane) = -5316.205869

O	-1.73590900	-2.22940200	-1.02109400
O	-3.14995500	-0.32365000	0.02564600
P	-1.60679400	-0.78271500	-0.26317900
O	-0.98202400	0.28152800	-1.10833500
C	-3.54665300	-2.13737200	-4.79257000
C	-4.31485000	-2.23370200	-3.63656400
C	-3.70000200	-2.34491900	-2.38115000
C	-1.50618000	-2.18062300	-3.43982400
C	-2.15508500	-2.14363200	-4.68582700
C	-4.00496300	-1.14020200	0.76757900
C	-4.61572300	-2.23813700	0.15906800
C	-5.34029300	-3.14055500	0.95517900
C	-5.54774100	-2.89264400	2.30745600
C	-5.03678000	-1.72176800	2.86606500
C	-4.25285300	-0.82765600	2.11919600
H	-1.54473800	-2.09437600	-5.58294300
H	-5.22798900	-1.49095100	3.90999400
C	-4.74243800	-2.64057400	-1.31040300
C	-6.00432200	-1.98708300	-1.97104400
H	-5.99276700	-0.91120400	-1.76152700
H	-6.94089300	-2.39424900	-1.57740300
H	-6.87720200	-4.27600300	-0.07022800
H	-5.62253800	-5.28112400	0.64701600
C	-2.31467200	-2.25201200	-2.28980500
H	-4.01776600	-2.06134900	-5.76939900
H	-6.11114100	-3.59094800	2.92119400
C	-5.82095700	-2.22317100	-3.48717800
H	-6.29837400	-1.44682400	-4.09595900
H	-6.25955800	-3.18154300	-3.79896400
C	-5.79889700	-4.32751500	0.13641000
C	-4.96964600	-4.18200700	-1.15673800
H	-3.99605600	-4.66878200	-1.02873100
H	-5.45088400	-4.62248600	-2.03554600
C	-3.78708300	0.43788800	2.77205400
C	-2.83349700	0.39552200	3.81737000
C	-4.40286000	1.66623200	2.42102000
C	-2.17007000	-0.81148700	4.20834000
C	-2.49227800	1.60954100	4.52599900
C	-4.04252500	2.87479500	3.12912800
C	-1.25766000	-0.82421300	5.22954800
H	-2.37274200	-1.71958400	3.65606500

C	-1.54342000	1.54992700	5.59565200
C	-3.09987600	2.81345500	4.16013700
C	-0.94560500	0.36834200	5.94246400
H	-0.74957100	-1.74967000	5.48312300
H	-1.31308300	2.46862800	6.13090300
H	-2.84654100	3.72284300	4.70231900
H	-0.22510200	0.33561600	6.75534200
C	-0.01171300	-2.16530300	-3.37634500
C	0.70373800	-1.02722500	-3.82336500
C	0.68729700	-3.31301900	-2.92744600
C	0.05830400	0.17370000	-4.26539300
C	2.14960300	-1.04926800	-3.83116300
C	2.13223200	-3.31075200	-2.91633900
C	0.78013400	1.24680700	-4.72172300
H	-1.02236600	0.23172900	-4.22098000
C	2.86461000	0.09373100	-4.31127500
C	2.82252500	-2.18458200	-3.37187700
C	2.20429100	1.20819500	-4.75362700
H	0.26012800	2.13993500	-5.05900800
H	3.95154900	0.05109700	-4.32345300
H	3.91083400	-2.19517500	-3.37571100
H	2.75975500	2.06536100	-5.12527800
C	-6.00802900	2.96746000	1.11087700
H	-6.77633000	3.01094000	0.34353800
C	-5.41169700	1.76982500	1.40957900
H	-5.71370900	0.87421700	0.87912100
C	-5.63795800	4.15688000	1.80132700
H	-6.12504300	5.09727800	1.55700400
C	-4.68114800	4.10678400	2.78021100
H	-4.39952500	5.00438700	3.32646800
C	0.73141700	-5.59840000	-2.06275900
H	0.20110100	-6.48959700	-1.73798700
C	2.15464700	-5.58197600	-2.03499400
H	2.69698200	-6.45586900	-1.68447700
C	2.83116300	-4.46961300	-2.45522000
H	3.91833000	-4.44497000	-2.44791100
C	0.02574700	-4.50706700	-2.49643800
H	-1.05719900	-4.54391200	-2.51944300
C	-0.34864700	3.95189600	-0.55396300
C	-0.85721600	3.18814600	0.71661200
H	-1.43239900	3.89481000	1.32801100
H	-1.54434200	2.40654400	0.38569700
C	0.16285500	2.55687800	1.61745900
C	0.66213600	3.04725500	-1.34871100

H	1.49443700	3.65387000	-1.70845700
H	0.15108300	2.61275100	-2.20786800
N	1.21509100	1.87371400	-0.64765600
C	2.49478500	1.70825900	-0.27026000
N	2.96617700	0.45194500	-0.16321800
C	4.25240800	0.08158100	0.32960400
C	4.34001800	-0.77004000	1.43294400
C	5.40793100	0.50802300	-0.32907500
C	5.59834700	-1.18230000	1.87728700
C	6.65649200	0.09724700	0.13430200
H	5.33084100	1.15028200	-1.19836900
C	6.75929400	-0.75051800	1.23815400
H	7.73141900	-1.07222400	1.59227100
C	7.89955900	0.50549600	-0.61235300
C	5.69822300	-2.04890700	3.10760200
F	8.21581800	-0.39124800	-1.57560400
F	8.96829000	0.59569100	0.20753700
F	7.74813800	1.70068100	-1.22266900
F	5.68645700	-1.30397700	4.23669500
F	6.84424100	-2.76610300	3.12029500
F	4.67086500	-2.91580300	3.19262700
S	3.40182100	3.08461100	0.27431900
H	3.43682500	-1.09491000	1.93924700
H	2.30423900	-0.33332100	-0.27090700
H	0.62078500	1.03881900	-0.80040700
C	1.15036200	3.19680800	2.35454100
H	1.05920200	4.28099200	2.45803000
H	2.12775500	3.22695700	1.39164000
N	-0.97927300	-1.12577500	1.19297500
S	0.48037800	-1.68163100	1.40869200
O	1.14420400	-1.04262200	2.56011500
O	1.30044900	-1.79501600	0.16876700
C	0.22584400	-3.45559100	1.94048200
F	-0.50011900	-3.49856800	3.06781500
F	1.41328300	-4.02237500	2.17357400
F	-0.41082600	-4.14125000	0.98997700
C	-1.55053800	4.29758600	-1.46052500
C	-1.36109900	4.53568500	-2.83422600
C	-2.84993700	4.44956700	-0.95529200
C	-2.42143800	4.89559400	-3.66553100
H	-0.36957000	4.45595500	-3.26846900
C	-3.91409500	4.80758600	-1.78568400
H	-3.06400000	4.27929900	0.09358400
C	-3.70846300	5.03137200	-3.14521100

H	-2.23695900	5.06971900	-4.72254300
H	-4.90828000	4.90166900	-1.35769400
H	-4.53767300	5.30698400	-3.79119300
C	0.33676500	5.30268200	-0.12211700
H	-0.37669300	5.82578800	0.53052100
H	1.22033200	5.07637300	0.47803100
C	0.74874200	6.23371000	-1.23230600
C	2.01580200	6.53105600	-1.54248100
H	2.82138300	6.05959900	-0.97723200
H	-0.05477300	6.70676200	-1.79539900
H	0.08208400	1.47773100	1.74454400
C	2.43710900	7.48744400	-2.62133900
H	3.02392200	8.31849100	-2.20697500
H	3.07905500	6.99334900	-3.36314800
H	1.57380500	7.91080700	-3.14584900
C	1.83796400	2.48138500	3.51056200
H	1.89241400	1.40389500	3.32864600
H	2.85169600	2.86414600	3.66669100
H	1.27054000	2.63211100	4.43585700

TS-EF-4RS

l imaginary frequency

H = -5315.353945

G = -5315.554544

E(M06-2X-DCM) = -5316.232789

E(M06-2X-cyclohexane) = -5316.204734

O	0.94111400	-2.92268300	-0.11941600
O	2.73320100	-1.07705300	-0.35956200
P	1.12225800	-1.29828700	-0.23728300
O	0.66795400	-0.57937700	0.99570300
C	2.84636100	-4.87200200	3.05782500
C	3.51969900	-4.63102800	1.86467600
C	2.86371200	-4.02916800	0.78006200
C	0.83724100	-3.83014700	2.12982100
C	1.50950600	-4.49009300	3.17174700
C	3.41547000	-1.57785900	-1.46959900
C	3.74790000	-2.92988500	-1.52392900
C	4.24786400	-3.45742700	-2.72527100
C	4.53675200	-2.62373400	-3.80062200
C	4.33134300	-1.24904500	-3.66928800
C	3.75586800	-0.69625400	-2.51430800
H	0.96918700	-4.68020800	4.09470300
H	4.59715700	-0.58162600	-4.48388100
C	3.77514700	-4.00987900	-0.44328800

C	5. 17617300	-4. 04021200	0. 26214700
H	5. 44095600	-3. 01889900	0. 55922800
H	5. 96736700	-4. 41133200	-0. 39641300
H	5. 43605200	-5. 26723900	-2. 55223300
H	3. 96994800	-5. 47606700	-3. 50314700
C	1. 54932400	-3. 59541300	0. 93798500
H	3. 35219600	-5. 34472100	3. 89598500
H	4. 93098700	-3. 02992300	-4. 72883700
C	4. 96679100	-4. 90662000	1. 52177300
H	5. 65089900	-4. 64287200	2. 33632400
H	5. 12860900	-5. 97230900	1. 30596000
C	4. 38268200	-4. 96275100	-2. 62704300
C	3. 60826800	-5. 28801000	-1. 32918200
H	2. 54432600	-5. 42280400	-1. 55522000
H	3. 96248700	-6. 19431700	-0. 82751800
C	3. 57095500	0. 78434500	-2. 39575100
C	2. 67111400	1. 46902700	-3. 24869200
C	4. 35273100	1. 50755100	-1. 45867700
C	1. 84376200	0. 79814500	-4. 20593700
C	2. 54917700	2. 90694700	-3. 14991200
C	4. 20440600	2. 94165700	-1. 35895900
C	0. 99063800	1. 49267700	-5. 02201700
H	1. 87192700	-0. 28329500	-4. 25485200
C	1. 64634700	3. 59401700	-4. 02145700
C	3. 30781700	3. 60110600	-2. 20416900
C	0. 89381900	2. 91058400	-4. 93837300
H	0. 36039300	0. 95358800	-5. 72302200
H	1. 57867500	4. 67672000	-3. 93996800
H	3. 19096200	4. 67917700	-2. 11784000
H	0. 21479100	3. 44379400	-5. 59896800
C	-0. 58646600	-3. 40992100	2. 32009900
C	-0. 89934200	-2. 38829500	3. 24947800
C	-1. 62004200	-4. 07127400	1. 61381500
C	0. 10356700	-1. 65337900	3. 96211900
C	-2. 28117000	-2. 03768900	3. 48748500
C	-2. 99623600	-3. 69507100	1. 84313800
C	-0. 22915700	-0. 67086800	4. 85854600
H	1. 14616100	-1. 87293900	3. 76694700
C	-2. 58662700	-1. 01401100	4. 44034000
C	-3. 28961200	-2. 69814200	2. 77873000
C	-1. 59463200	-0. 34967200	5. 11001500
H	0. 55578700	-0. 12321800	5. 37395200
H	-3. 63285200	-0. 77642300	4. 62178700
H	-4. 32998500	-2. 43456900	2. 96112800

H	-1.84170300	0.42576200	5.83035100
C	6.04666700	1.61083200	0.30342100
H	6.76609100	1.10796500	0.94403900
C	5.31541500	0.88498400	-0.59987100
H	5.46884400	-0.18539100	-0.67421500
C	5.87662400	3.01974900	0.41328900
H	6.46180200	3.57751800	1.13951100
C	4.98502900	3.66332400	-0.40152600
H	4.84263500	4.73855800	-0.33013100
C	-2.39001600	-5.74615500	0.01061000
H	-2.16888600	-6.54265400	-0.69481300
C	-3.74237400	-5.35659200	0.22588900
H	-4.53907700	-5.85400400	-0.32077300
C	-4.03361700	-4.36175200	1.11915600
H	-5.06198100	-4.05310100	1.29124100
C	-1.36797900	-5.12757200	0.68113700
H	-0.34437100	-5.43953500	0.50819300
N	0.50963200	-0.91890200	-1.68645800
S	-1.00767000	-1.00617500	-2.09292700
O	-1.37905700	0.03982200	-3.06127000
O	-1.95365100	-1.19737900	-0.95455400
C	-1.15360200	-2.58987800	-3.07597400
F	-0.32675700	-2.54509200	-4.12793200
F	-2.41027200	-2.72030800	-3.52112100
F	-0.84655900	-3.65005700	-2.32680900
C	-5.15049300	1.01602200	-0.08626200
C	-4.52482200	1.15623600	-1.50771000
H	-5.33437400	1.43279200	-2.19815100
H	-4.13699900	0.18184400	-1.81304300
C	-3.42041400	2.14953900	-1.69533600
C	-4.00409600	0.77337400	0.97062300
H	-4.21638700	1.33614000	1.88150700
H	-3.97460700	-0.28865400	1.22281900
N	-2.63079700	1.09362800	0.54984500
C	-1.85750400	2.07684200	1.07043300
N	-0.54570500	1.82675400	1.16837800
C	0.49025800	2.72047100	1.55673000
C	0.67949900	3.96692700	0.95825000
C	1.38759500	2.26230600	2.52671400
C	1.74711500	4.76723900	1.36586700
C	2.45017200	3.07225100	2.92106800
H	1.24732900	1.27835500	2.95920800
C	2.63204000	4.33244600	2.35182900
H	3.45941000	4.95922100	2.66133300

C	3.44528400	2.56193500	3.93090600
C	1.92316800	6.12972100	0.74967300
F	2.89019500	1.65863200	4.77085600
F	4.49734700	1.95855400	3.33834800
F	3.94217200	3.56692100	4.68732300
F	1.20894200	7.07419600	1.40077900
F	3.21578600	6.53005000	0.77174100
F	1.51701600	6.15296500	-0.54181600
S	-2.58125600	3.60642900	1.44220800
H	0.01593700	4.30438900	0.17337100
H	-0.21478700	0.83776400	1.07516300
H	-2.14806100	0.27745100	0.14335400
C	-3.48059200	3.52289200	-1.48783400
H	-4.47985700	3.95189300	-1.38307500
H	-3.16440400	3.54173100	-0.17811200
C	-5.97222500	2.28462100	0.32634900
H	-5.30064800	3.12929500	0.49959000
H	-6.41927200	2.06297300	1.30577600
C	-6.10980300	-0.19430500	-0.03744000
C	-6.50332200	-0.92103900	-1.16896900
C	-6.64076600	-0.59118800	1.20384400
C	-7.38453700	-2.00131900	-1.06612900
H	-6.12396900	-0.66243500	-2.15087200
C	-7.51706700	-1.66958500	1.31177400
H	-6.36899000	-0.05099200	2.10732600
C	-7.89517400	-2.38293500	0.17228500
H	-7.66608300	-2.54469100	-1.96405000
H	-7.90805400	-1.94816500	2.28688100
H	-8.58051300	-3.22227300	0.25089200
C	-7.06859700	2.67403100	-0.62815600
C	-7.29655600	3.91633000	-1.06842700
H	-6.64268300	4.72445100	-0.73217400
H	-7.73728300	1.87316700	-0.94718200
H	-2.49364100	1.73538500	-2.09422300
C	-8.41756300	4.31864000	-1.98370000
H	-8.03617800	4.79172800	-2.89855300
H	-9.02763000	3.45721800	-2.27511900
H	-9.07641400	5.05420400	-1.50293300
C	-2.44114700	4.44406700	-2.11607600
H	-2.27391500	5.33445900	-1.50075400
H	-1.48298400	3.93192800	-2.25425800
H	-2.78109300	4.78169200	-3.10196500

l imaginary frequency

H = -5315.351724

G = -5315.552694

E(M06-2X-DCM) = -5316.232179

E(M06-2X-cyclohexane) = -5316.203410

O	0.82049500	-2.93468800	-0.07400500
O	2.71083400	-1.18947700	-0.31333700
P	1.08895600	-1.32413600	-0.21212100
O	0.65430600	-0.56328200	1.00258500
C	2.57002600	-4.92819000	3.16490800
C	3.27423300	-4.74168600	1.97984900
C	2.66763600	-4.12506400	0.87500100
C	0.63246900	-3.80013500	2.18660700
C	1.25284200	-4.47672600	3.24987600
C	3.38175700	-1.74425800	-1.40464900
C	3.64350000	-3.11258000	-1.43166200
C	4.13328500	-3.68604800	-2.61602300
C	4.48128600	-2.88723100	-3.70029800
C	4.34592900	-1.50170200	-3.59492100
C	3.78312200	-0.89982100	-2.45836000
H	0.68842800	-4.62397800	4.16621900
H	4.65827100	-0.86314800	-4.41611300
C	3.59792800	-4.17372000	-0.33313300
C	4.98422200	-4.26394600	0.39572900
H	5.29684800	-3.25262000	0.68023200
H	5.76531900	-4.68666400	-0.24350500
H	5.22358600	-5.55115800	-2.39399300
H	3.76328600	-5.70094500	-3.36477500
C	1.37518100	-3.62149500	1.00379500
H	3.03709600	-5.41229400	4.01892000
H	4.86769100	-3.32934600	-4.61529300
C	4.71064500	-5.09651100	1.66592900
H	5.39422200	-4.85364600	2.48738800
H	4.82123600	-6.17266700	1.47072400
C	4.18857900	-5.19435800	-2.49076200
C	3.37881600	-5.45680500	-1.20034800
H	2.31290500	-5.54087800	-1.44120400
H	3.67814700	-6.37117000	-0.67799400
C	3.67474000	0.59027000	-2.36755700
C	2.82418100	1.30599000	-3.24523000
C	4.48067800	1.28791400	-1.43165500
C	1.97613900	0.66253300	-4.20318300
C	2.77709000	2.74986300	-3.17294100
C	4.40743100	2.72942100	-1.35905100

C	1. 17243100	1. 38627200	-5. 04367400
H	1. 94788300	-0. 41959300	-4. 23312500
C	1. 92382300	3. 46777700	-4. 06922500
C	3. 55869500	3. 41995500	-2. 22853400
C	1. 14924100	2. 80858400	-4. 98552300
H	0. 52467900	0. 86861600	-5. 74488800
H	1. 91210100	4. 55380300	-4. 00705400
H	3. 49873100	4. 50415100	-2. 16326600
H	0. 50868800	3. 36488000	-5. 66524800
C	-0. 77067000	-3. 30470200	2. 34618600
C	-1. 04575300	-2. 25418900	3. 25510500
C	-1. 82519600	-3. 92308200	1. 63190000
C	-0. 01813100	-1. 55992100	3. 97330100
C	-2. 41152600	-1. 83023900	3. 46480800
C	-3. 18376400	-3. 47332400	1. 83199200
C	-0. 31454200	-0. 54782600	4. 84932600
H	1. 01491300	-1. 83489100	3. 79868500
C	-2. 67953300	-0. 77790600	4. 39753700
C	-3. 44089700	-2. 44904900	2. 74854500
C	-1. 66572300	-0. 15418000	5. 07357500
H	0. 48901700	-0. 03254000	5. 36939800
H	-3. 71507400	-0. 48499600	4. 55818800
H	-4. 46925100	-2. 13017500	2. 90934900
H	-1. 88437300	0. 64385500	5. 77824600
C	6. 15376000	1. 33326800	0. 35264200
H	6. 83667400	0. 80471600	1. 01226300
C	5. 39705800	0. 63087300	-0. 54821500
H	5. 49416400	-0. 44731800	-0. 60153500
C	6. 05763200	2. 75099800	0. 43531800
H	6. 66193400	3. 29011900	1. 15995900
C	5. 21243100	3. 42598100	-0. 40321700
H	5. 12635800	4. 50832600	-0. 35259500
C	-2. 65394500	-5. 57988600	0. 03933100
H	-2. 46261300	-6. 39726500	-0. 65076500
C	-3. 98770100	-5. 11774800	0. 22516000
H	-4. 79976700	-5. 58128200	-0. 32862100
C	-4. 24207700	-4. 09605800	1. 09919700
H	-5. 25572500	-3. 73190600	1. 24851700
C	-1. 61255600	-5. 00490900	0. 71886700
H	-0. 60373100	-5. 37184400	0. 56832700
N	0. 51873700	-0. 93513000	-1. 67620600
S	-0. 99442200	-0. 94838500	-2. 10474900
O	-1. 29629200	0. 10198300	-3. 09263900
O	-1. 96641000	-1. 07352900	-0. 97889300

C	-1.20986500	-2.53582200	-3.06869700
F	-0.36874500	-2.54822100	-4.11017600
F	-2.46594500	-2.60725700	-3.52853600
F	-0.96739400	-3.59970900	-2.30148000
C	-5.07672700	1.29218900	-0.17527500
C	-4.41506200	1.34591000	-1.58520500
H	-5.19422200	1.60386900	-2.31576500
H	-4.05119800	0.34599900	-1.83298500
C	-3.27445900	2.29548600	-1.78727500
C	-3.95423200	1.03181700	0.90339700
H	-4.14496600	1.63758100	1.79109600
H	-3.97953500	-0.02061500	1.19334600
N	-2.56337200	1.27021700	0.48272500
C	-1.74119900	2.22072900	0.99236500
N	-0.44621600	1.90118700	1.10929700
C	0.63159100	2.74568400	1.49500500
C	0.89450000	3.96849800	0.87603200
C	1.48992100	2.26004400	2.48661600
C	1.99683500	4.71976900	1.28454800
C	2.58808000	3.02084600	2.88141900
H	1.29218600	1.29345900	2.93543600
C	2.84383200	4.25852300	2.29155600
H	3.69845800	4.84718500	2.60188400
C	3.54049100	2.47944700	3.91599200
C	2.25193300	6.05960400	0.64672500
F	2.92752100	1.62078400	4.76241300
F	4.56963100	1.81321800	3.35125100
F	4.07595400	3.47184200	4.66269700
F	1.58300000	7.05233300	1.27362600
F	3.56389000	6.39067800	0.67608600
F	1.86059600	6.08139600	-0.64929400
S	-2.38363300	3.79433100	1.32296300
H	0.26046300	4.32499700	0.07534700
H	-0.16725700	0.89449400	1.03969600
H	-2.12036400	0.42127500	0.09822800
C	-3.27140700	3.67682100	-1.60903200
H	-4.24505300	4.16323700	-1.51135300
H	-2.95512900	3.71832000	-0.31041300
C	-5.83829700	2.61757900	0.18342000
H	-5.10321300	3.40922100	0.36106500
H	-6.33484800	2.45865500	1.14706700
C	-6.09617000	0.13651200	-0.10012600
C	-6.52508100	-0.59470800	-1.21459300
C	-6.64916300	-0.20167600	1.14840800

C	-7.46123600	-1.62482000	-1.08899800
H	-6.13203300	-0.37896800	-2.20143900
C	-7.58202900	-1.22911100	1.27965400
H	-6.35077400	0.34522200	2.03957100
C	-7.99436600	-1.94913100	0.15638200
H	-7.76937600	-2.17399700	-1.97462800
H	-7.98901000	-1.46323100	2.25997200
H	-8.72299400	-2.74931900	0.25268200
C	-6.86061700	3.07543800	-0.82216700
C	-8.18397500	3.03216500	-0.64135200
H	-8.57057900	2.62812800	0.29577200
H	-6.48294600	3.48166600	-1.76312100
H	-2.36428200	1.83686300	-2.17605400
C	-9.21075400	3.49741700	-1.63240300
H	-9.84380200	4.28782700	-1.20717800
H	-8.74601400	3.88851300	-2.54391000
H	-9.88329700	2.67746800	-1.91784200
C	-2.19236600	4.53181500	-2.26563400
H	-1.98884800	5.43351400	-1.67865600
H	-1.25695800	3.97449900	-2.38280100
H	-2.51530900	4.85078700	-3.26328800

TS-EF-4RS-2

l imaginary frequency

H = -5315.353454

G = -5315.553239

E(M06-2X-DCM) = -5316.229978

E(M06-2X-cyclohexane) = -5316.202693

O	0.73442600	-2.95699100	0.15033000
O	2.61791500	-1.22065200	-0.18811000
P	0.99457200	-1.36351100	-0.12988400
O	0.50708500	-0.49199500	0.98491900
C	2.43408200	-4.65554400	3.57922300
C	3.15885700	-4.56676900	2.39528300
C	2.57116000	-4.04787200	1.23154500
C	0.50979300	-3.62755100	2.47301100
C	1.11381700	-4.20634100	3.60149700
C	3.32775900	-1.85268500	-1.21061700
C	3.59313200	-3.21751000	-1.12637700
C	4.11547200	-3.87744700	-2.25008600
C	4.49362600	-3.16103300	-3.38097300
C	4.35775800	-1.77128500	-3.38232900
C	3.76239700	-1.08761600	-2.31046700
H	0.53271300	-4.27925400	4.51632100

H	4.69616800	-1.19506900	-4.23857600
C	3.52555700	-4.18994000	0.04972500
C	4.89762100	-4.21527400	0.81062800
H	5.20212300	-3.18290800	1.01793100
H	5.69213300	-4.68536800	0.22315200
H	5.20035800	-5.71885300	-1.86263500
H	3.76161400	-5.94417200	-2.85053900
C	1.27373700	-3.54338500	1.29347500
H	2.88733500	-5.06297800	4.47941900
H	4.90534000	-3.66931600	-4.24936100
C	4.60116900	-4.94237100	2.13863300
H	5.26900100	-4.63225600	2.95031600
H	4.71584000	-6.03061400	2.03329400
C	4.16783500	-5.37189800	-2.00858100
C	3.32960500	-5.53728400	-0.71963000
H	2.26965900	-5.64509500	-0.97673300
H	3.62017900	-6.40693700	-0.12146300
C	3.65739900	0.40532300	-2.32685000
C	2.83792900	1.06158800	-3.27738500
C	4.43601300	1.16358400	-1.41497200
C	2.01637400	0.35590800	-4.21440000
C	2.79597700	2.50724200	-3.30596300
C	4.36556600	2.60681900	-1.44195900
C	1.24293100	1.02185500	-5.12809600
H	1.98531200	-0.72565800	-4.17080200
C	1.97657600	3.16375300	-4.27797000
C	3.54892300	3.23851100	-2.38393100
C	1.22719600	2.44486100	-5.17042800
H	0.61503800	0.45881100	-5.81214600
H	1.97193000	4.25156000	-4.29462700
H	3.49060900	4.32477100	-2.39296100
H	0.61342300	2.95475000	-5.90878300
C	-0.90320500	-3.14218600	2.56697400
C	-1.20876500	-2.01593400	3.36875000
C	-1.93911300	-3.85461000	1.91616800
C	-0.20288800	-1.23871800	4.03026100
C	-2.58487000	-1.60301500	3.52700400
C	-3.31025900	-3.42828300	2.07840000
C	-0.52929000	-0.15602600	4.80537700
H	0.83723100	-1.50963100	3.89515600
C	-2.88384200	-0.46988000	4.34866600
C	-3.59615500	-2.31820700	2.87867800
C	-1.88982500	0.23316200	4.97390600
H	0.25801800	0.41964600	5.28479100

H	-3.92605600	-0.18093600	4.46581900
H	-4.63239000	-2.01139300	3.00943500
H	-2.13120500	1.09107100	5.59589900
C	6.04920400	1.32680900	0.41694200
H	6.70806100	0.84297600	1.13289200
C	5.32086800	0.56639300	-0.45981500
H	5.41657400	-0.51296100	-0.43772600
C	5.95488500	2.74689200	0.40119800
H	6.53663600	3.33296000	1.10762900
C	5.14055400	3.36510600	-0.50859400
H	5.05692200	4.44847100	-0.53275600
C	-2.72067000	-5.69300200	0.50777700
H	-2.50562400	-6.56925200	-0.09778900
C	-4.06961200	-5.26599100	0.66810300
H	-4.87077300	-5.82250800	0.18859000
C	-4.35188200	-4.16620500	1.43323100
H	-5.37781100	-3.83239100	1.56897800
C	-1.69562700	-5.01440500	1.11257600
H	-0.67547500	-5.35900300	0.98788500
N	0.47402400	-1.12850000	-1.64722600
S	-1.02928900	-1.15714300	-2.10310900
O	-1.29551400	-0.20904200	-3.19862700
O	-2.01975900	-1.14271300	-0.98400400
C	-1.27456800	-2.83406900	-2.89257900
F	-0.42919800	-2.97742300	-3.91943400
F	-2.53018300	-2.92710200	-3.34895200
F	-1.05984900	-3.81210000	-2.01100700
C	-5.04869800	1.44657600	-0.91841900
C	-4.22412400	1.51958200	-2.26385700
H	-4.93202200	1.83990500	-3.04162400
H	-3.89895200	0.51045100	-2.52136000
C	-3.01884000	2.40106500	-2.32843700
C	-4.08821800	1.26394900	0.31679100
H	-4.36232200	1.98855000	1.08322200
H	-4.21396600	0.26858600	0.74572200
N	-2.64481500	1.40428200	0.05986100
C	-1.84234100	2.35045200	0.60844600
N	-0.57135900	1.99610700	0.85159200
C	0.50569900	2.82728500	1.26647900
C	0.83247600	4.02014000	0.61950700
C	1.30219000	2.35777500	2.31621200
C	1.93169100	4.75966700	1.05605500
C	2.40005700	3.10539600	2.73690300
H	1.05939000	1.41234900	2.78687400

C	2. 71667600	4. 31506800	2. 11890700
H	3. 57055900	4. 89323600	2. 45026400
C	3. 29260500	2. 57761000	3. 82999600
C	2. 24943600	6. 06848200	0. 38345700
F	2. 62721900	1. 75279300	4. 67111000
F	4. 33504900	1. 87903300	3. 33250300
F	3. 81061700	3. 58148500	4. 57377000
F	1. 56220600	7. 09645000	0. 92835400
F	3. 56291800	6. 37984900	0. 47828600
F	1. 93620600	6. 04441000	-0. 93437600
S	-2. 45235600	3. 95513000	0. 83104000
H	0. 24931700	4. 36355600	-0. 22392800
H	-0. 32077500	0. 98190300	0. 85555700
H	-2. 20272200	0. 51079700	-0. 20703900
C	-2. 97708200	3. 78908900	-2. 18943600
H	-3. 93668100	4. 30825300	-2. 26018800
H	-2. 83939200	3. 85417700	-0. 88623000
C	-5. 85457300	2. 76874500	-0. 70577900
H	-6. 46703100	2. 95275900	-1. 59949400
H	-5. 14679500	3. 59886900	-0. 64366400
C	-5. 97853200	0. 22199900	-1. 09441900
C	-5. 45222000	-1. 07870800	-1. 00046300
C	-7. 32822800	0. 34958600	-1. 45676600
C	-6. 24907000	-2. 20003300	-1. 22961400
H	-4. 40031800	-1. 23457900	-0. 77917900
C	-8. 12918200	-0. 77249700	-1. 68334600
H	-7. 78036100	1. 32854400	-1. 56986000
C	-7. 59564600	-2. 05405200	-1. 56539400
H	-5. 80385000	-3. 18744700	-1. 14813900
H	-9. 17267300	-0. 63631300	-1. 95543300
H	-8. 21771800	-2. 92735600	-1. 74221500
C	-6. 71897100	2. 80876800	0. 53062600
C	-6. 61244700	3. 73040600	1. 49400000
H	-5. 84540100	4. 50158100	1. 40403800
H	-7. 47942800	2. 03520700	0. 62991900
H	-2. 08562200	1. 88512800	-2. 55656700
C	-7. 47874300	3. 80277500	2. 71840800
H	-8. 02242300	4. 75618400	2. 76301500
H	-8. 21399300	2. 99145000	2. 74216300
H	-6. 87569800	3. 74473800	3. 63437500
C	-1. 78413400	4. 57875700	-2. 72032400
H	-1. 62468700	5. 49365200	-2. 14049100
H	-0. 86559700	3. 98333900	-2. 69180700
H	-1. 95690300	4. 87014500	-3. 76251200

TS-EF-4RS-3

1 imaginary frequency

H = -5315.350764

G = -5315.551404

E(M06-2X-DCM) = -5316.229399

E(M06-2X-cyclohexane) = -5316.201336

O	0.73973700	-2.95947600	0.16640400
O	2.66400800	-1.24820400	-0.03542800
P	1.03862900	-1.36968600	-0.09685100
O	0.48531800	-0.49368800	0.98463500
C	2.13010000	-4.64664100	3.73710800
C	2.95153300	-4.57530000	2.61681100
C	2.46745000	-4.06147600	1.40409300
C	0.31648700	-3.60584200	2.46804400
C	0.81781600	-4.18237800	3.64675600
C	3.44062000	-1.90127700	-0.99416800
C	3.68564800	-3.26745600	-0.87183900
C	4.28845500	-3.94711200	-1.94237600
C	4.75961800	-3.25018600	-3.05014400
C	4.63479300	-1.86001200	-3.08185000
C	3.96421500	-1.15628100	-2.06896800
H	0.16258700	-4.24020600	4.51119400
H	5.04185400	-1.29877500	-3.91789500
C	3.51410300	-4.22477100	0.30643700
C	4.81851900	-4.25391900	1.17780400
H	5.11452800	-3.22215200	1.39986100
H	5.65433400	-4.73667400	0.66228100
H	5.32342700	-5.79046200	-1.44429400
H	3.96807900	-6.01913200	-2.54333000
C	1.17559300	-3.54245300	1.35428000
H	2.50263300	-5.05113300	4.67489400
H	5.23336200	-3.77413200	-3.87660100
C	4.40677300	-4.96528500	2.48367900
H	5.00792100	-4.65220400	3.34487100
H	4.52041500	-6.05539300	2.39863000
C	4.30899400	-5.43839200	-1.67850200
C	3.36769600	-5.58005700	-0.46027100
H	2.33102500	-5.68145000	-0.80120800
H	3.60002600	-6.44464300	0.16985300
C	3.87142700	0.33665500	-2.12032200
C	3.13344400	0.97831000	-3.14485300
C	4.58388900	1.10831000	-1.16677700
C	2.38132800	0.25885100	-4.12848500

C	3. 10587800	2. 42321100	-3. 20595700
C	4. 52924200	2. 55111200	-1. 22954300
C	1. 68720800	0. 91113500	-5. 11284600
H	2. 33586500	-0. 82122600	-4. 06482600
C	2. 36887400	3. 06510800	-4. 25075400
C	3. 79270100	3. 16838700	-2. 24426200
C	1. 68575900	2. 33299900	-5. 18442500
H	1. 10895600	0. 33836400	-5. 83170700
H	2. 37183700	4. 15236700	-4. 28746300
H	3. 74597700	4. 25455500	-2. 28147900
H	1. 13385800	2. 83160900	-5. 97726800
C	-1. 08884600	-3. 09272800	2. 43879000
C	-1. 43969800	-1. 96059600	3. 21355900
C	-2. 07469600	-3. 77330300	1. 68428500
C	-0. 48015500	-1. 20555300	3. 96382600
C	-2. 81410600	-1. 51475300	3. 24515500
C	-3. 44099900	-3. 30365400	1. 70555300
C	-0. 84976300	-0. 11514700	4. 70818500
H	0. 56163800	-1. 49909300	3. 92054600
C	-3. 16058500	-0. 37850400	4. 04386300
C	-3. 77454100	-2. 19630500	2. 49144800
C	-2. 21146600	0. 30231500	4. 75758500
H	-0. 09555900	0. 44402400	5. 25594300
H	-4. 20300800	-0. 06770100	4. 07096400
H	-4. 81017500	-1. 86239100	2. 52155900
H	-2. 48918000	1. 16374200	5. 35930700
C	6. 05456200	1. 29888200	0. 77901100
H	6. 65234800	0. 82564100	1. 55329100
C	5. 38747000	0. 52522400	-0. 13417100
H	5. 47050200	-0. 55415400	-0. 08160100
C	5. 97560500	2. 71906100	0. 72575900
H	6. 50787200	3. 31577300	1. 46170000
C	5. 23854400	3. 32348900	-0. 25632100
H	5. 16752900	4. 40671800	-0. 31067900
C	-2. 76157600	-5. 57258400	0. 18117200
H	-2. 51261400	-6. 45217300	-0. 40640200
C	-4. 10172700	-5. 09213000	0. 18945300
H	-4. 86060000	-5. 60404200	-0. 39618100
C	-4. 42878900	-3. 99148100	0. 93371800
H	-5. 44767400	-3. 61203000	0. 94548100
C	-1. 78569200	-4. 93756300	0. 90310500
H	-0. 77122400	-5. 31917500	0. 88850100
N	0. 63299600	-1. 12506700	-1. 64450000
S	-0. 82790200	-1. 15183500	-2. 22710300

O	-0.99329500	-0.20137100	-3.34044800
O	-1.91476300	-1.14192300	-1.20412900
C	-0.99069200	-2.82518900	-3.04451500
F	-0.04557100	-2.96182000	-3.98267700
F	-2.19295100	-2.91857900	-3.62681400
F	-0.86272900	-3.80821200	-2.15186600
C	-5.03934700	1.35053900	-1.01724600
C	-4.22360700	1.30824900	-2.35312400
H	-4.90158900	1.59533600	-3.16786900
H	-3.91033800	0.27626600	-2.53059300
C	-3.00633600	2.17533300	-2.47168000
C	-4.05887000	1.15242700	0.19569400
H	-4.34490800	1.81792000	1.01186600
H	-4.13106500	0.12269400	0.55071000
N	-2.62139900	1.33989200	-0.07515100
C	-1.83967100	2.31215400	0.45427900
N	-0.57677800	1.98086500	0.75288300
C	0.47298600	2.83616500	1.18938100
C	0.83209600	4.00184900	0.51130000
C	1.20553900	2.41744100	2.30489700
C	1.89936000	4.76721800	0.98198000
C	2.27168200	3.19030400	2.75952800
H	0.93722400	1.49210900	2.80137600
C	2.61945800	4.37425900	2.10934200
H	3.44819200	4.97283400	2.46717600
C	3.09364800	2.71679600	3.93028600
C	2.25150400	6.04983600	0.27645600
F	2.37201000	1.93892500	4.76942600
F	4.15962000	1.98997800	3.53384900
F	3.57155500	3.75607000	4.65187000
F	1.52932400	7.09425000	0.73901000
F	3.55585100	6.37268800	0.43648000
F	2.01680900	5.97126900	-1.05487300
S	-2.46874900	3.92233600	0.56906600
H	0.29963400	4.30335600	-0.38061900
H	-0.31808400	0.96760800	0.79993300
H	-2.15777300	0.45346600	-0.33086800
C	-2.95332900	3.56523200	-2.43436700
H	-3.90492500	4.09457800	-2.52714400
H	-2.82121100	3.72444800	-1.10132100
C	-5.79384200	2.72761600	-0.89576300
H	-6.34605800	2.87415600	-1.83503000
H	-5.05468400	3.52798500	-0.82391300
C	-6.09400300	0.22289000	-1.02327000

C	-6.60810200	-0.31970600	-2.21042900
C	-6.62508900	-0.25956300	0.18672600
C	-7.59424600	-1.30848700	-2.19272000
H	-6.23934100	0.01267800	-3.17445100
C	-7.61305700	-1.24429300	0.20915300
H	-6.27989200	0.14804800	1.13145200
C	-8.10182100	-1.77863200	-0.98340600
H	-7.96047500	-1.71183200	-3.13297700
H	-8.00287800	-1.58918100	1.16346300
H	-8.86851800	-2.54824100	-0.96917000
C	-6.75224700	2.87149200	0.25749900
C	-6.56561800	3.68967700	1.29967900
H	-5.65264100	4.28578200	1.34460900
H	-7.66553700	2.27970400	0.21075300
H	-2.08027000	1.63962100	-2.68188100
C	-7.53041700	3.87180600	2.43614200
H	-7.86810400	4.91474600	2.50476500
H	-8.41485300	3.23599100	2.32190700
H	-7.05984400	3.63356400	3.39952500
C	-1.74796500	4.30750900	-3.00064800
H	-1.57900000	5.25265100	-2.47389800
H	-0.83715800	3.70339000	-2.93304200
H	-1.91079700	4.54249100	-4.05881300

TS-EF-4RS-4

l imaginary frequency

H = -5315.348918

G = -5315.550223

E(M06-2X-DCM) = -5316.228372

E(M06-2X-cyclohexane) = -5316.199680

O	0.79970000	-2.94810600	0.13406800
O	2.71042600	-1.21834100	-0.04027200
P	1.08661600	-1.35297500	-0.10822800
O	0.52341900	-0.49584400	0.98354000
C	2.19008000	-4.66725000	3.68944400
C	3.01556500	-4.57467800	2.57369000
C	2.53203100	-4.05022800	1.36529100
C	0.37270400	-3.62629400	2.42580000
C	0.87422700	-4.21325600	3.59932200
C	3.49586400	-1.85326200	-1.00406200
C	3.75310500	-3.21840100	-0.89604300
C	4.36652000	-3.88027900	-1.97169300
C	4.83553600	-3.16652700	-3.06960800
C	4.69681400	-1.77744000	-3.08679800

C	4. 01517800	-1. 09142500	-2. 06911800
H	0. 21607900	-4. 28732400	4. 46029000
H	5. 10102900	-1. 20320800	-3. 91535500
C	3. 58498500	-4. 19086800	0. 27034500
C	4. 88577100	-4. 21868000	1. 14711700
H	5. 17128600	-3. 18703400	1. 38303800
H	5. 72825100	-4. 68739800	0. 62950300
H	5. 41620500	-5. 71962000	-1. 48975400
H	4. 06816500	-5. 94811700	-2. 59778500
C	1. 23576900	-3. 54206200	1. 31646600
H	2. 56224800	-5. 08012800	4. 62371100
H	5. 31772800	-3. 67667000	-3. 89980500
C	4. 47486800	-4. 94975400	2. 44230500
H	5. 06931300	-4. 64179800	3. 30997200
H	4. 59889000	-6. 03765100	2. 34446000
C	4. 39967500	-5. 37421400	-1. 72478100
C	3. 45408600	-5. 53836300	-0. 51275000
H	2. 41993500	-5. 64482900	-0. 85974500
H	3. 69110900	-6. 40817100	0. 10836100
C	3. 90422000	0. 40067800	-2. 10671000
C	3. 16358000	1. 04239700	-3. 12938500
C	4. 60092200	1. 17249600	-1. 14174600
C	2. 42691000	0. 32275100	-4. 12452300
C	3. 11679400	2. 48733200	-3. 17652400
C	4. 52664200	2. 61499500	-1. 19042400
C	1. 73019900	0. 97535400	-5. 10682000
H	2. 39518000	-0. 75839400	-4. 07165400
C	2. 37764800	3. 12956200	-4. 21959300
C	3. 78737700	3. 23220600	-2. 20318100
C	1. 71019600	2. 39767900	-5. 16464600
H	1. 16402100	0. 40204900	-5. 83482500
H	2. 36599700	4. 21706400	-4. 24548100
H	3. 72556700	4. 31798600	-2. 22969300
H	1. 15630800	2. 89662600	-5. 95586600
C	-1. 03652800	-3. 12361600	2. 39865900
C	-1. 39828900	-2. 00546200	3. 18878200
C	-2. 01516900	-3. 80060400	1. 63161500
C	-0. 44615700	-1. 25210200	3. 95013400
C	-2. 77662900	-1. 57234100	3. 22515100
C	-3. 38536600	-3. 34239800	1. 65692300
C	-0. 82604800	-0. 17541400	4. 70919600
H	0. 59827500	-1. 53548400	3. 90330400
C	-3. 13404200	-0. 45121800	4. 04029800
C	-3. 73004500	-2. 25055900	2. 45956700

C	-2.19164000	0.22842200	4.76410500
H	-0.07733200	0.38301500	5.26525500
H	-4.17968300	-0.15170200	4.07256400
H	-4.76850800	-1.92585500	2.49182100
H	-2.47771200	1.07817900	5.37837900
C	6.05850500	1.36381800	0.81377600
H	6.65880400	0.89116000	1.58646700
C	5.40705400	0.59022700	-0.11068400
H	5.50488600	-0.48838200	-0.06856200
C	5.95993200	2.78323800	0.77444300
H	6.47966400	3.37972300	1.51944600
C	5.21979600	3.38727000	-0.20554800
H	5.13399200	4.46993500	-0.24948600
C	-2.68430300	-5.58123500	0.09870700
H	-2.42698300	-6.44941200	-0.50208800
C	-4.02828400	-5.11154600	0.11106300
H	-4.78157700	-5.62018600	-0.48453000
C	-4.36605000	-4.02546600	0.87177800
H	-5.38797100	-3.65423400	0.88738000
C	-1.71512600	-4.95018800	0.83306500
H	-0.69764800	-5.32354600	0.81490600
N	0.68307300	-1.09113900	-1.65332600
S	-0.77483400	-1.12867500	-2.24310500
O	-0.94797200	-0.16332100	-3.34222900
O	-1.86608700	-1.14907800	-1.22494300
C	-0.91108500	-2.79142900	-3.08636700
F	0.03952700	-2.90082600	-4.02258000
F	-2.10960400	-2.89269900	-3.67482400
F	-0.77288900	-3.78592500	-2.20798400
C	-5.03304200	1.32944900	-0.92605200
C	-4.25810600	1.30336000	-2.28805200
H	-4.95608000	1.62121700	-3.07390100
H	-3.96975700	0.26988300	-2.49724900
C	-3.02526600	2.14791600	-2.41930500
C	-4.01682200	1.07243600	0.24629300
H	-4.28229000	1.67043400	1.11793400
H	-4.06900900	0.01958600	0.53000400
N	-2.58801500	1.29729800	-0.03956500
C	-1.82478400	2.28015600	0.49725600
N	-0.55441900	1.97237200	0.78672900
C	0.47831300	2.84393300	1.23092400
C	0.81677400	4.02011700	0.56055800
C	1.21675800	2.43114900	2.34458300
C	1.87079900	4.80047900	1.03628100

C	2.26847800	3.21995100	2.80546000
H	0.96372500	1.49840000	2.83535000
C	2.59646300	4.41324100	2.16218100
H	3.41460400	5.02380700	2.52416300
C	3.09639900	2.75377100	3.97500100
C	2.20410000	6.09168600	0.33714200
F	2.38499100	1.96258700	4.81033200
F	4.17271500	2.04335900	3.57654400
F	3.55911500	3.79682900	4.70079500
F	1.47036900	7.12414500	0.80783700
F	3.50487400	6.42976700	0.49521600
F	1.96658000	6.01735100	-0.99386300
S	-2.49374100	3.87234200	0.63297000
H	0.27953100	4.31728500	-0.33004600
H	-0.27668400	0.96315900	0.82139300
H	-2.10821100	0.42469300	-0.31143200
C	-2.94596900	3.53638200	-2.38162000
H	-3.88607700	4.08520300	-2.47910700
H	-2.82783200	3.68951900	-1.04172100
C	-5.77504500	2.71009300	-0.77431200
H	-6.45497100	2.80502000	-1.62984000
H	-5.03530800	3.51043900	-0.85881700
C	-6.10359400	0.21872900	-0.91625000
C	-6.62760400	-0.33555600	-2.09330600
C	-6.63539200	-0.23788500	0.30264600
C	-7.62438700	-1.31325600	-2.05694600
H	-6.25873200	-0.02187800	-3.06360200
C	-7.63055100	-1.21440800	0.34423500
H	-6.28095700	0.17886700	1.23947500
C	-8.13021900	-1.76087400	-0.83836300
H	-7.99891500	-1.72676600	-2.98952700
H	-8.01900200	-1.54196900	1.30517000
H	-8.90418600	-2.52285500	-0.80932300
C	-6.54728500	2.94556300	0.49638100
C	-7.87814700	3.03958600	0.57233500
H	-8.46602500	2.90294100	-0.33722300
H	-5.96127500	3.09764800	1.40424000
H	-2.11018000	1.59691400	-2.63696800
C	-8.65711000	3.32140900	1.82416500
H	-9.35759000	2.50472200	2.04531900
H	-7.99878100	3.44946300	2.69010800
H	-9.26188800	4.23228400	1.71987000
C	-1.72321900	4.25582400	-2.93888600
H	-1.53823600	5.19583200	-2.40823200

H	-0.82509000	3.63332800	-2.86947900
H	-1.87579200	4.49799900	-3.99697200

TS-EF-4RS-5

l imaginary frequency

H = -5315.341139

G = -5315.544139

E(M06-2X-DCM) = -5316.227407

E(M06-2X-cyclohexane) = -5316.197104

O	2.83810400	-1.64964900	-0.07350100
O	2.24357900	0.53813100	-1.32307400
P	1.61931900	-0.58263400	-0.29942600
O	1.22350800	0.17576100	0.93520800
C	6.35104900	-0.27105900	1.73137100
C	6.14213800	-0.10165800	0.36615700
C	5.00073200	-0.63354100	-0.25343400
C	4.21316900	-1.45012400	1.91191000
C	5.40543300	-0.97113300	2.48149700
C	2.68828300	0.17649700	-2.59359900
C	3.95323000	-0.39241200	-2.74021300
C	4.32966800	-0.90104100	-3.99386500
C	3.51202900	-0.73016700	-5.10547900
C	2.30608200	-0.04473800	-4.96047800
C	1.85761600	0.40853500	-3.70888800
H	5.57422200	-1.13871300	3.54120000
H	1.67489500	0.12787700	-5.82720600
C	5.12766200	-0.51059000	-1.76912700
C	6.06546000	0.74137500	-1.86334500
H	5.45392000	1.64705800	-1.77066300
H	6.59520700	0.79654200	-2.81929000
H	6.46553500	-1.02341200	-4.36052400
H	5.65141700	-2.58302900	-4.41625000
C	4.02026200	-1.23457700	0.53316400
H	7.24214200	0.12606900	2.21121500
H	3.80733600	-1.11597700	-6.07796100
C	7.00750600	0.61855300	-0.64555900
H	7.35980600	1.59095700	-0.28224300
H	7.90429600	0.03295900	-0.89185400
C	5.66072000	-1.61519800	-3.90209400
C	5.86075800	-1.75356400	-2.37749500
H	5.36450900	-2.66287900	-2.01977100
H	6.91239100	-1.80673200	-2.07889500
C	0.55572300	1.14360500	-3.62271900
C	-0.65557700	0.48524500	-3.95073900

C	0.54662700	2.52489700	-3.30105400
C	-0.71933800	-0.91264000	-4.25378400
C	-1.89613100	1.22895300	-3.96273600
C	-0.70457300	3.25067500	-3.29633800
C	-1.90460200	-1.52151000	-4.57097300
H	0.18566200	-1.50178900	-4.18894400
C	-3.11203300	0.55624900	-4.30569900
C	-1.88789000	2.58585500	-3.63041100
C	-3.11915300	-0.77933600	-4.60951800
H	-1.92389900	-2.58907000	-4.76777600
H	-4.03618100	1.12976100	-4.31255300
H	-2.82428700	3.14062800	-3.63865200
H	-4.05131100	-1.28077500	-4.85112300
C	3.21552000	-2.17936800	2.75404500
C	2.58532600	-1.51939200	3.83842800
C	2.94087500	-3.54639100	2.49922800
C	2.81431100	-0.14065600	4.15493700
C	1.66064800	-2.24798700	4.67807900
C	1.99182900	-4.25162800	3.32920900
C	2.21962200	0.45496200	5.23832700
H	3.47156300	0.43989600	3.51836100
C	1.05075200	-1.58581100	5.78969100
C	1.38113500	-3.58653000	4.39416900
C	1.32664900	-0.27526600	6.07420400
H	2.43063100	1.49781000	5.46175700
H	0.36554600	-2.15660500	6.41248800
H	0.67469200	-4.12635300	5.02153700
H	0.86999100	0.21036100	6.93293000
C	1.69404700	4.59694700	-2.68459200
H	2.61363800	5.12538100	-2.44959300
C	1.73638500	3.26285900	-2.99722800
H	2.69054400	2.74953100	-3.02194800
C	0.45615600	5.29991600	-2.66243600
H	0.44144800	6.35783800	-2.41447600
C	-0.70575500	4.64247800	-2.96513100
H	-1.65751400	5.16899800	-2.96579600
C	3.28937700	-5.60814400	1.23378700
H	3.79229000	-6.14415000	0.43331000
C	2.33206200	-6.28873400	2.03785600
H	2.10580200	-7.33277200	1.83930100
C	1.70779500	-5.62625900	3.05860900
H	0.98000600	-6.13337400	3.68746700
C	3.58458300	-4.28949000	1.45878000
H	4.32510600	-3.79522600	0.84095500

N	0.49796800	-1.37164600	-1.14130900
S	-0.40290000	-2.54307300	-0.55605500
O	-1.82163800	-2.27251500	-0.89169900
O	-0.10588300	-2.97313500	0.81791200
C	0.05969500	-4.00334200	-1.62499900
F	-0.15888400	-3.75107800	-2.92378900
F	-0.67604500	-5.06107000	-1.26756900
F	1.35325700	-4.29387000	-1.45788800
C	0.08964400	3.67758400	1.95074600
C	0.28810700	2.62080800	3.10546700
H	0.56386800	3.18803300	4.00489000
H	1.13616000	1.98855000	2.84231800
C	-0.85338500	1.71444900	3.44052600
C	-0.54154400	2.98517200	0.68686700
H	-1.31306400	3.63542200	0.27538500
H	0.21585500	2.84551900	-0.08436400
N	-1.13411000	1.64506900	0.89318200
C	-2.44685300	1.34963700	0.76196600
N	-2.78840500	0.13662600	0.29003400
C	-4.11060800	-0.40240300	0.22216200
C	-4.88995600	-0.58289600	1.36685000
C	-4.58610100	-0.80845000	-1.02294000
C	-6.16095400	-1.13949100	1.25171000
C	-5.86102600	-1.37151100	-1.12355800
H	-3.96299400	-0.69212200	-1.90312500
C	-6.65659900	-1.53549900	0.00656200
H	-7.64329600	-1.97465500	-0.07602100
C	-6.35483700	-1.78698900	-2.48558800
C	-7.03275700	-1.27242200	2.47258000
F	-5.57556700	-2.74650500	-3.02869900
F	-7.61720800	-2.26055300	-2.44864300
F	-6.34075200	-0.74260600	-3.35071300
F	-7.87054800	-0.21767300	2.60072600
F	-7.80232100	-2.38011000	2.41860500
F	-6.30273900	-1.33528400	3.60863300
S	-3.62502400	2.47274300	1.35300400
H	-4.50692000	-0.30049400	2.33835900
H	-2.09671900	-0.45311400	-0.19200100
H	-0.43178200	0.89067000	0.77754400
C	-2.08798500	2.08035500	3.97495800
H	-2.14558300	3.08548800	4.40096800
H	-2.73415600	2.34454500	2.84054900
C	-0.86138200	4.82311300	2.41967700
H	-0.44636200	5.26157600	3.33828300

H	-1.82431600	4.39072000	2.69780600
C	1.51553900	4.20364400	1.64999600
C	1.97275800	5.45021200	2.10458700
C	2.44074000	3.37517800	0.99089400
C	3.28828900	5.86680800	1.88451000
H	1.31149700	6.12229000	2.63937900
C	3.75495800	3.78707400	0.77514900
H	2.15102200	2.38224000	0.66301900
C	4.18662600	5.03937000	1.21431200
H	3.60553100	6.84210100	2.24466900
H	4.44234200	3.11416900	0.26942200
H	5.21055600	5.36175500	1.04463300
C	-1.12280200	5.90532200	1.39996500
C	-2.34172600	6.31328000	1.03170300
H	-3.21586600	5.83089700	1.47198200
H	-0.25435400	6.38123200	0.94665300
H	-0.66953100	0.65227700	3.28393800
C	-2.62266700	7.40605600	0.04092000
H	-3.22388600	7.03368400	-0.79947100
H	-3.19987200	8.22010600	0.50010800
H	-1.69832000	7.83243400	-0.36329800
C	-2.97151100	1.04317000	4.65904800
H	-4.02919600	1.31893900	4.60014300
H	-2.84731700	0.05523100	4.20307100
H	-2.70693000	0.95482500	5.71874300

TS-EF-4RS-6

l imaginary frequency

H = -5315.338884

G = -5315.544729

E(M06-2X-DCM) = -5316.223307

E(M06-2X-cyclohexane) = -5316.192541

O	2.72208300	-1.74873600	-0.15347600
O	2.37311200	0.57167300	-1.26416800
P	1.61875900	-0.55489700	-0.34145500
O	1.22703600	0.13260600	0.93274900
C	6.28228300	-0.86900100	1.85845600
C	6.13473800	-0.56296400	0.50934000
C	4.97289500	-0.93557600	-0.18270000
C	4.04235300	-1.85932700	1.87879700
C	5.25479500	-1.54510900	2.51733200
C	2.83651800	0.24886200	-2.53835500
C	4.04743600	-0.42967700	-2.67888600
C	4.42454200	-0.89343900	-3.95007500

C	3.66850400	-0.58492800	-5.07533000
C	2.52952400	0.20630600	-4.92834500
C	2.08316100	0.63178600	-3.66706600
H	5.37564500	-1.82453900	3.55986300
H	1.95251300	0.49296300	-5.80276800
C	5.16782600	-0.71409500	-1.67900600
C	6.20909500	0.45590500	-1.64673400
H	5.67162000	1.39989300	-1.49984600
H	6.77720200	0.53608400	-2.57877400
H	6.55353100	-1.17440700	-4.25608000
H	5.61610900	-2.65308100	-4.44027400
C	3.91397800	-1.50326800	0.52137800
H	7.18858600	-0.59864600	2.39474100
H	3.96352400	-0.94154300	-6.05896700
C	7.09170200	0.16103100	-0.41321300
H	7.50227100	1.07115200	0.03917200
H	7.94961900	-0.47340800	-0.67666300
C	5.68634500	-1.72389700	-3.86329800
C	5.81759600	-1.97351400	-2.34617600
H	5.23479600	-2.85820000	-2.06523600
H	6.84916600	-2.13461300	-2.01802200
C	0.88035000	1.52127400	-3.58592900
C	-0.40289800	1.02849900	-3.92422100
C	1.05408500	2.89497100	-3.28071000
C	-0.63941800	-0.34392300	-4.25469100
C	-1.53657200	1.92690500	-3.93469100
C	-0.09061000	3.77886100	-3.27925900
C	-1.88938400	-0.79121500	-4.59108200
H	0.18525400	-1.04158400	-4.20052300
C	-2.82542300	1.41992700	-4.29472500
C	-1.35291700	3.27077900	-3.59963900
C	-2.99946300	0.10122300	-4.62278600
H	-2.04189400	-1.84371000	-4.80901900
H	-3.66636100	2.10978800	-4.30532900
H	-2.20901100	3.94288600	-3.60972500
H	-3.98448400	-0.27263700	-4.88655700
C	2.96255300	-2.57366500	2.62695700
C	2.37678900	-1.97679500	3.77188600
C	2.56773200	-3.87531900	2.22686800
C	2.73270700	-0.67070000	4.24242500
C	1.37094200	-2.69886400	4.51935200
C	1.53881000	-4.56995800	2.96576000
C	2.18168900	-0.14396400	5.38301600
H	3.45415400	-0.09102500	3.67885700

C	0.80831000	-2.10614200	5.69349200
C	0.97057100	-3.96573600	4.08883000
C	1.20662500	-0.86938200	6.12572000
H	2.49001700	0.84150800	5.72374500
H	0.06075600	-2.67237200	6.24470700
H	0.20434700	-4.49932900	4.64771100
H	0.78520000	-0.43949400	7.03088300
C	2.47859300	4.81491100	-2.76256600
H	3.46850200	5.22760100	-2.58644800
C	2.33657900	3.47519000	-3.01588600
H	3.21275500	2.83742600	-3.03665600
C	1.34399100	5.67582200	-2.73686900
H	1.47405000	6.73562100	-2.53382500
C	0.09720000	5.16612000	-2.98460400
H	-0.77672200	5.81370500	-2.98348700
C	2.75440900	-5.82068400	0.75890600
H	3.22512500	-6.31700400	-0.08547700
C	1.71811300	-6.48593100	1.47268100
H	1.40046700	-7.47768100	1.16257300
C	1.13396800	-5.87583600	2.54824900
H	0.34770900	-6.37374000	3.11058200
C	3.16503800	-4.56604800	1.12455800
H	3.96392400	-4.08441700	0.57331100
N	0.46629100	-1.18431100	-1.27847500
S	-0.49318900	-2.37383400	-0.85258400
O	-1.88327000	-2.03209100	-1.24253400
O	-0.29248900	-2.93030500	0.49364900
C	-0.02070400	-3.75254600	-2.02148800
F	-0.19375100	-3.38704400	-3.30150900
F	-0.78636700	-4.82131000	-1.77894400
F	1.26149200	-4.08346100	-1.84234600
C	0.08841200	3.34820100	2.45037300
C	0.28181900	2.09796700	3.37494500
H	0.54333200	2.45414600	4.37787600
H	1.12557900	1.52313800	2.98975800
C	-0.87388700	1.15995200	3.53757200
C	-0.48745800	2.87351800	1.07046300
H	-1.18520200	3.61728800	0.68303700
H	0.33382600	2.76181000	0.36210200
N	-1.14754300	1.54865400	1.04148900
C	-2.46488900	1.32119700	0.85949300
N	-2.84163800	0.21921700	0.18749100
C	-4.17149200	-0.28240200	0.04152600
C	-4.96933200	-0.59715000	1.14390100

C	-4.63338100	-0.52350400	-1.25084700
C	-6.24372400	-1.12040300	0.94219400
C	-5.90998100	-1.05914800	-1.43864900
H	-3.99625400	-0.30225400	-2.10037500
C	-6.72394200	-1.35442700	-0.34906600
H	-7.71198000	-1.77203300	-0.49938700
C	-6.38392100	-1.30000400	-2.84890200
C	-7.13433300	-1.39608200	2.12523100
F	-5.57676000	-2.16065600	-3.50574200
F	-7.63479100	-1.80194500	-2.88936300
F	-6.38612100	-0.15001100	-3.56731700
F	-7.96501800	-0.35724200	2.37253700
F	-7.91192600	-2.48066100	1.92272600
F	-6.42149600	-1.60760300	3.25422100
S	-3.60847500	2.36183400	1.64317300
H	-4.59821500	-0.44647700	2.14848600
H	-2.15898200	-0.31489400	-0.36853200
H	-0.46387600	0.80421900	0.81231000
C	-2.09437900	1.44121000	4.14023900
H	-2.14133300	2.35961000	4.73080300
H	-2.75324400	1.94060700	3.05061600
C	-0.86734500	4.39836500	3.12682600
H	-0.46978100	4.58741400	4.13453900
H	-1.86205600	3.96495100	3.24598400
C	1.45984600	4.03642600	2.26401700
C	1.80496400	4.68502200	1.06731400
C	2.37685800	4.11656200	3.32557900
C	3.01829000	5.36226000	0.93319700
H	1.12792800	4.68599600	0.21996200
C	3.59080100	4.79076100	3.19404100
H	2.15714000	3.64755700	4.27896600
C	3.92110600	5.41693800	1.99302500
H	3.25073500	5.84480600	-0.01148600
H	4.27796600	4.82255300	4.03558000
H	4.86687200	5.94125300	1.88648900
C	-1.00465500	5.71267200	2.40347800
C	-2.13939200	6.16513500	1.85879200
H	-3.03567300	5.54552300	1.91535300
H	-0.10991100	6.33137000	2.34522200
H	-0.70301300	0.14023200	3.19506700
C	-2.29348200	7.48808400	1.16466800
H	-2.63540300	7.35606300	0.12924700
H	-3.04673700	8.11253200	1.66401400
H	-1.35082400	8.04521600	1.14362500

C	-3.00270800	0.31707800	4.62074500
H	-4.05548300	0.61774100	4.60966800
H	-2.89224500	-0.57559100	3.99593400
H	-2.74768700	0.03419700	5.64843800

TS-EF-4RS-7

l imaginary frequency

H = -5315.337228

G = -5315.541868

E(M06-2X-DCM) = -5316.222456

E(M06-2X-cyclohexane) = -5316.191342

O	2.72056300	-1.79997400	0.05628900
O	2.32849800	0.32253300	-1.38464900
P	1.60241400	-0.65516200	-0.28721100
O	1.23203200	0.21720800	0.87579200
C	6.28285200	-0.58027900	1.87761900
C	6.11860000	-0.47676800	0.49997300
C	4.95863700	-0.96704200	-0.11809400
C	4.06234000	-1.59569500	2.06625800
C	5.27397500	-1.17144600	2.63914500
C	2.78110200	-0.18564300	-2.60062200
C	4.00515300	-0.85300100	-2.65228400
C	4.38096300	-1.49477000	-3.84378800
C	3.60712300	-1.37568100	-4.99274300
C	2.44972100	-0.59879900	-4.95119000
C	2.00500300	0.00236800	-3.76272800
H	5.40866400	-1.29388000	3.70987300
H	1.85659200	-0.46243800	-5.85080000
C	5.13860000	-0.96314200	-1.63285000
C	6.15527300	0.21910500	-1.78216200
H	5.59946500	1.16378200	-1.76842700
H	6.71459000	0.17372700	-2.72182800
H	6.51330100	-1.77173100	-4.12881300
H	5.60909400	-3.28146100	-4.08106500
C	3.91608000	-1.44306700	0.67302800
H	7.18803000	-0.21830100	2.35898400
H	3.90152700	-1.86919000	-5.91553400
C	7.05317000	0.12387600	-0.52818700
H	7.44781700	1.09801000	-0.21699000
H	7.92235500	-0.52491100	-0.70583100
C	5.66223000	-2.27554900	-3.64916800
C	5.81111100	-2.29396900	-2.11343100
H	5.25086100	-3.13935200	-1.69783300
H	6.84863200	-2.38299200	-1.77668800

C	0.77536700	0.85762700	-3.79871200
C	-0.49265900	0.28074600	-4.05217900
C	0.90433400	2.26540000	-3.69036800
C	-0.68635600	-1.13182100	-4.17925100
C	-1.65546200	1.13157700	-4.18048800
C	-0.26867600	3.10327900	-3.80699100
C	-1.92278100	-1.66215900	-4.43495200
H	0.16054400	-1.78849100	-4.03216600
C	-2.92940200	0.53725800	-4.44974900
C	-1.51451100	2.51474200	-4.04304200
C	-3.06169000	-0.81984600	-4.58223100
H	-2.04223400	-2.73928700	-4.49776700
H	-3.79392200	1.19003400	-4.54842200
H	-2.39213100	3.15088700	-4.14267500
H	-4.03586700	-1.25892500	-4.77559600
C	3.00102800	-2.21135700	2.92114500
C	2.41188700	-1.46400000	3.97198600
C	2.62744000	-3.56416100	2.71909900
C	2.74550000	-0.09669800	4.24222800
C	1.42570500	-2.08672400	4.82719600
C	1.61681500	-4.16111400	3.56140500
C	2.19272000	0.58137100	5.29901100
H	3.45155700	0.40643400	3.59220400
C	0.86097500	-1.33904000	5.90814600
C	1.04586100	-3.40950700	4.59017600
C	1.23824500	-0.04532500	6.15057300
H	2.48449300	1.61137500	5.48956000
H	0.12889300	-1.83201300	6.54396100
H	0.29366600	-3.86891400	5.22832700
H	0.81578900	0.50477700	6.98759000
C	2.26509600	4.28368900	-3.44798700
H	3.24012500	4.74819500	-3.32822800
C	2.16692100	2.91815000	-3.51335000
H	3.06337700	2.31251800	-3.44714400
C	1.10347200	5.10262900	-3.54200500
H	1.19901300	6.18424700	-3.49183300
C	-0.12596100	4.52363000	-3.71238300
H	-1.02011200	5.13662700	-3.80179000
C	2.83954900	-5.69970200	1.54900900
H	3.31362300	-6.30599400	0.78182000
C	1.82069600	-6.27131300	2.36209700
H	1.51923200	-7.30305200	2.20313400
C	1.23305100	-5.52070600	3.34277400
H	0.46006600	-5.94449900	3.97933700

C	3. 22959300	-4. 39818300	1. 72367700
H	4. 01570500	-3. 98856700	1. 10050700
N	0. 43936500	-1. 42632000	-1. 09579500
S	-0. 54642500	-2. 48939700	-0. 45124300
O	-1. 93392300	-2. 18203200	-0. 87901700
O	-0. 33892700	-2. 80014600	0. 97138500
C	-0. 12916100	-4. 06941300	-1. 35651700
F	-0. 29860500	-3. 93403200	-2. 68074800
F	-0. 92789700	-5. 05075900	-0. 92465500
F	1. 14254100	-4. 40477000	-1. 12161900
C	0. 12722900	3. 68308400	1. 89632600
C	0. 36763100	2. 59665300	3. 00060300
H	0. 60842800	3. 11573800	3. 93570500
H	1. 23501700	2. 00261900	2. 70767800
C	-0. 75168400	1. 64573600	3. 29763400
C	-0. 42785300	2. 97896800	0. 60780300
H	-1. 10184100	3. 64227500	0. 06666500
H	0. 41475300	2. 74161100	-0. 04321400
N	-1. 10764200	1. 67614600	0. 78247700
C	-2. 43241300	1. 45145900	0. 67087500
N	-2. 84891200	0. 27450800	0. 17380800
C	-4. 19473500	-0. 20301200	0. 11929800
C	-4. 97788700	-0. 34416000	1. 26698400
C	-4. 69037300	-0. 59598000	-1. 12222300
C	-6. 27118800	-0. 84787700	1. 15741400
C	-5. 98685200	-1. 10823000	-1. 21672400
H	-4. 06569200	-0. 50730000	-2. 00481900
C	-6. 78567200	-1. 23224000	-0. 08375600
H	-7. 79002900	-1. 63060800	-0. 16131900
C	-6. 49512300	-1. 52614100	-2. 57267400
C	-7. 14592800	-0. 93768300	2. 38044100
F	-5. 80493300	-2. 57924600	-3. 06195900
F	-7. 79810100	-1. 87257800	-2. 54487200
F	-6. 36105300	-0. 52416300	-3. 47587800
F	-7. 96159600	0. 13637800	2. 48549400
F	-7. 93829400	-2. 03006900	2. 34745600
F	-6. 41806300	-0. 99318500	3. 51811500
S	-3. 52893700	2. 61939900	1. 33556600
H	-4. 58129000	-0. 07451200	2. 23621400
H	-2. 18959600	-0. 35899800	-0. 30150700
H	-0. 44031400	0. 89402800	0. 65358700
C	-1. 96776300	1. 95612500	3. 89331200
H	-2. 03007700	2. 92634900	4. 39263300
H	-2. 65424100	2. 34612300	2. 76302800

C	-0.83908600	4.79802100	2.44662200
H	-0.34075200	5.24878700	3.31347800
H	-1.75476300	4.32712900	2.81193700
C	1.46628100	4.37776400	1.57015200
C	1.69325900	4.95488000	0.31048600
C	2.46865300	4.53497200	2.54078600
C	2.87462400	5.64251500	0.03029400
H	0.94780200	4.88067500	-0.47370200
C	3.65103100	5.22239100	2.26403300
H	2.34491200	4.11588900	3.53370100
C	3.86204300	5.78033000	1.00420000
H	3.01653300	6.07032400	-0.95804800
H	4.40803300	5.31596800	3.03839400
H	4.78268800	6.31448000	0.78519100
C	-1.23550200	5.88519700	1.48360100
C	-0.81071600	7.15060000	1.54602000
H	-0.10349600	7.42845500	2.32963300
H	-1.95113300	5.61144100	0.70712200
H	-0.55402500	0.60092000	3.06352800
C	-1.22538200	8.25045700	0.61232900
H	-1.69465500	9.08044300	1.15769500
H	-0.35636000	8.67167900	0.08893800
H	-1.93664500	7.89451400	-0.14069400
C	-2.84133500	0.86356200	4.49394900
H	-3.90018700	1.14235100	4.48221800
H	-2.72547000	-0.07966000	3.94966600
H	-2.55707600	0.67931000	5.53631000

TS-EF-4RS-8

l imaginary frequency

H = -5315.341663

G = -5315.545123

E(M06-2X-DCM) = -5316.225610

E(M06-2X-cyclohexane) = -5316.194838

O	2.79381800	-1.21742600	1.21695100
O	2.22186800	-0.90023800	-1.29122900
P	1.59551900	-0.72859300	0.21487800
O	1.22234300	0.71706000	0.35496600
C	6.35803000	0.97203500	1.26588200
C	6.13068000	0.00838300	0.28862300
C	4.97362900	-0.78428600	0.32440300
C	4.20097600	0.43740800	2.29447900
C	5.41268200	1.14984900	2.27667800
C	2.65441400	-2.14251700	-1.74974800

C	3.91335900	-2.61231400	-1.37399700
C	4.27958900	-3.92514200	-1.71354900
C	3.45725000	-4.71076300	-2.51322000
C	2.25768700	-4.17555500	-2.98093900
C	1.82223500	-2.89449000	-2.60460100
H	5.59720500	1.87269000	3.06600600
H	1.62272900	-4.76308100	-3.63760000
C	5.09091800	-1.91463700	-0.69341300
C	6.03415200	-1.23636200	-1.74414100
H	5.42875000	-0.60085500	-2.40073600
H	6.55456200	-1.96628600	-2.37200200
H	6.41210500	-4.30345700	-1.83939300
H	5.59539400	-5.28034400	-0.62373900
C	3.99094000	-0.51041900	1.27267400
H	7.26343200	1.57397900	1.25399500
H	3.74501000	-5.72432700	-2.78093800
C	6.98816400	-0.35869900	-0.90347800
H	7.34349900	0.52208600	-1.45080800
H	7.88227200	-0.91906300	-0.59609500
C	5.60897600	-4.28812600	-1.08908800
C	5.81639200	-3.15270800	-0.06508000
H	5.31881300	-3.40894500	0.87726900
H	6.86914600	-2.95213700	0.15674900
C	0.53441300	-2.37480400	-3.16608400
C	-0.69334700	-2.99507100	-2.82785500
C	0.55967900	-1.33291400	-4.12740500
C	-0.78611500	-4.05154500	-1.86618300
C	-1.91821500	-2.55380800	-3.45830500
C	-0.67551800	-0.88660300	-4.73323400
C	-1.98437400	-4.64716900	-1.57409700
H	0.10804500	-4.35505200	-1.33813000
C	-3.14930200	-3.20317500	-3.12511100
C	-1.87837100	-1.50539300	-4.38091500
C	-3.18359100	-4.22824000	-2.21722300
H	-2.02633600	-5.42934800	-0.82242800
H	-4.06214900	-2.86189200	-3.60792900
H	-2.80285000	-1.17626400	-4.85172200
H	-4.12616800	-4.70422000	-1.96514500
C	3.20253900	0.67849100	3.38108200
C	2.62598600	1.96366400	3.54289600
C	2.87415200	-0.36346300	4.28488000
C	2.91919400	3.06849400	2.67830600
C	1.69578500	2.19892800	4.62478500
C	1.91900900	-0.12032800	5.34103100

C	2. 38012100	4. 31153500	2. 89375000
H	3. 58325400	2. 91012800	1. 83673800
C	1. 14187300	3. 50563900	4. 80336700
C	1. 35764600	1. 15013900	5. 48252500
C	1. 47893400	4. 54015000	3. 97259700
H	2. 64208900	5. 13522900	2. 23356700
H	0. 44969600	3. 65959300	5. 62820700
H	0. 64636100	1. 32937500	6. 28625500
H	1. 06422700	5. 53239300	4. 13067900
C	1. 76900700	0. 26804800	-5. 52697300
H	2. 70867400	0. 70607000	-5. 85186500
C	1. 77317400	-0. 71593200	-4. 57280300
H	2. 71454900	-1. 05114100	-4. 15309000
C	0. 54690600	0. 72003700	-6. 10226700
H	0. 56187100	1. 49802800	-6. 86140500
C	-0. 63876600	0. 15768200	-5. 71054900
H	-1. 57882600	0. 47997600	-6. 15282900
C	3. 12548100	-2. 65075500	5. 10940300
H	3. 59428600	-3. 62837400	5. 03564600
C	2. 15986500	-2. 41294600	6. 12774100
H	1. 89272500	-3. 21130100	6. 81470700
C	1. 58001700	-1. 17934000	6. 23945100
H	0. 84761700	-0. 97759500	7. 01739700
C	3. 47098100	-1. 66321200	4. 22508700
H	4. 21712700	-1. 86422300	3. 46546000
N	0. 45350800	-1. 85954700	0. 34142400
S	-0. 51697500	-2. 00512500	1. 58742500
O	-1. 92272100	-2. 06657100	1. 10968300
O	-0. 24563800	-1. 13568800	2. 74185200
C	-0. 16528400	-3. 73576100	2. 19480600
F	-0. 36577200	-4. 64616700	1. 23096600
F	-0. 97661400	-4. 01585200	3. 22021500
F	1. 10317000	-3. 82069500	2. 60509000
C	0. 21794700	3. 69843500	-1. 59309500
C	0. 32043500	3. 86523800	-0. 04666400
H	0. 63824400	4. 89703000	0. 15491900
H	1. 09325300	3. 18801500	0. 31949800
C	-0. 91247100	3. 61672800	0. 76112300
C	-0. 38851200	2. 27944300	-1. 92073600
H	-1. 05873300	2. 34588300	-2. 77885000
H	0. 42710900	1. 59807800	-2. 16796000
N	-1. 11247600	1. 60330500	-0. 82485900
C	-2. 44039400	1. 37115200	-0. 77482500
N	-2. 87674800	0. 27631400	-0. 12719800

C	-4.23317800	-0.05273900	0.17544400
C	-5.05874700	0.80846100	0.90281100
C	-4.70061600	-1.30533100	-0.21843700
C	-6.36365100	0.42419100	1.19789400
C	-6.01110400	-1.68063300	0.08992400
H	-4.04437500	-1.98184100	-0.75539500
C	-6.85095700	-0.82091100	0.79150500
H	-7.86509900	-1.11746400	1.02993900
C	-6.49637900	-3.03183300	-0.36885100
C	-7.27875100	1.37625800	1.92222200
F	-5.75542900	-4.03258200	0.15322800
F	-7.78168600	-3.25602700	-0.02746200
F	-6.41102300	-3.15090700	-1.71733000
F	-8.06064000	2.06521200	1.05972700
F	-8.10613400	0.72647800	2.76813200
F	-6.58902200	2.28837000	2.64373000
S	-3.52287600	2.57327200	-1.40076200
H	-4.68637500	1.76480400	1.24310500
H	-2.22424900	-0.48408500	0.12185700
H	-0.46317300	1.02172700	-0.26411500
C	-2.11191800	4.31631500	0.68873700
H	-2.07464000	5.26713800	0.15179200
H	-2.70754600	3.60756800	-0.30097900
C	-0.66366500	4.80970200	-2.25947900
H	-1.71473600	4.67031500	-1.99675300
H	-0.60919600	4.63899700	-3.34395100
C	1.62369900	3.79580000	-2.22618000
C	1.78312500	3.48000900	-3.58656000
C	2.75779200	4.23083400	-1.52615600
C	3.01928900	3.59669900	-4.21931500
H	0.93543200	3.12655200	-4.16724200
C	3.99836800	4.35021800	-2.15796200
H	2.69433100	4.47841300	-0.47282900
C	4.13616100	4.03692000	-3.50810500
H	3.10663500	3.34285100	-5.27223600
H	4.85730800	4.68872300	-1.58456700
H	5.10030800	4.13153200	-4.00018400
C	-0.23824600	6.22423000	-1.97130100
C	-1.06345400	7.21461800	-1.61374200
H	-2.12955200	7.00118300	-1.50513900
H	0.82163700	6.44633000	-2.10281600
H	-0.82994700	2.83516500	1.51628700
C	-0.65289700	8.63959100	-1.37347500
H	-1.16449100	9.32121800	-2.06628700

H	-0.91903800	8.96752000	-0.35955400
H	0.42626700	8.77399400	-1.50217100
C	-3.11848100	4.25302400	1.83055600
H	-4.14357700	4.39190700	1.47166700
H	-3.06512300	3.29279700	2.35479900
H	-2.91400500	5.04194200	2.56340400

TS-EF-4RS-9

1 imaginary frequency

H = -5315.339304

G = -5315.543723

E(M06-2X-DCM) = -5316.224989

E(M06-2X-cyclohexane) = -5316.193165

O	2.65727800	-1.51080300	1.12364700
O	2.15745800	-0.88065700	-1.34066500
P	1.51062700	-0.84338500	0.16556200
O	1.21696700	0.59682500	0.46405100
C	6.34823800	0.42791600	1.46769800
C	6.08175800	-0.40360000	0.38473100
C	4.87734300	-1.11982600	0.31488200
C	4.14106900	-0.07894500	2.39952000
C	5.39490000	0.55177300	2.47898100
C	2.52324600	-2.08783300	-1.93214400
C	3.74259600	-2.67568700	-1.59400700
C	4.03487900	-3.96248500	-2.07516000
C	3.18337100	-4.59929900	-2.97089000
C	2.02943100	-3.93974100	-3.39237500
C	1.66528000	-2.68418400	-2.87920600
H	5.60761900	1.16832900	3.34741400
H	1.37417500	-4.40807500	-4.12098400
C	4.94604700	-2.13457400	-0.82237000
C	5.95070600	-1.40411600	-1.77673800
H	5.39927400	-0.66171300	-2.36516300
H	6.43799500	-2.09053200	-2.47617600
H	6.14221300	-4.45919600	-2.21270600
H	5.24125900	-5.51193100	-1.12685500
C	3.89395400	-0.89129500	1.27443100
H	7.28930700	0.96817800	1.53627800
H	3.41408300	-5.59248900	-3.34790500
C	6.93952000	-0.68876100	-0.82934500
H	7.35983500	0.22336800	-1.26859200
H	7.79065900	-1.33593700	-0.57504500
C	5.32582800	-4.47677200	-1.47689900
C	5.58109900	-3.47860400	-0.32821600

H	5.04949600	-3.80693800	0.57225500
H	6.63932800	-3.37091600	-0.07079900
C	0.42443600	-2.02364000	-3.39682100
C	-0.84645100	-2.59797400	-3.14889000
C	0.53509600	-0.88419100	-4.23335400
C	-1.02539200	-3.74768100	-2.31478000
C	-2.02771400	-2.01087400	-3.74254300
C	-0.65664700	-0.29441700	-4.80238800
C	-2.26437100	-4.29402500	-2.10908200
H	-0.16345500	-4.16553600	-1.81191900
C	-3.30367600	-2.61315400	-3.50274000
C	-1.90293600	-0.87023800	-4.53960700
C	-3.42115400	-3.72940500	-2.71760800
H	-2.37091300	-5.15127000	-1.45154600
H	-4.18285000	-2.16209900	-3.95718600
H	-2.79487600	-0.43149900	-4.98301700
H	-4.39665900	-4.16931700	-2.53478000
C	3.13694600	0.10319300	3.49234800
C	2.64071400	1.39731500	3.79184000
C	2.72244500	-1.01017200	4.26630700
C	3.02354300	2.57123000	3.06411600
C	1.70393100	1.56975200	4.87995300
C	1.76114200	-0.82545200	5.32872000
C	2.56206200	3.81512500	3.41352000
H	3.69398400	2.46585400	2.21933700
C	1.23217100	2.88181300	5.19957500
C	1.27968100	0.45523200	5.60657000
C	1.65420200	3.97934800	4.49848900
H	2.89241400	4.68901200	2.85657600
H	0.53382900	2.98698000	6.02689300
H	0.56376100	0.58905300	6.41502400
H	1.30221800	4.97277600	4.76461500
C	1.87136200	0.78346400	-5.42395600
H	2.84310200	1.19484500	-5.68244100
C	1.79385700	-0.29991900	-4.58799400
H	2.70335800	-0.73946700	-4.19518600
C	0.69237400	1.37434200	-5.96207300
H	0.77199600	2.23033100	-6.62745500
C	-0.53406400	0.84852300	-5.65424500
H	-1.44255000	1.27795500	-6.07072700
C	2.80801900	-3.38761200	4.82755400
H	3.21497900	-4.37943700	4.64979300
C	1.83626000	-3.20329100	5.85112100
H	1.50268600	-4.05489900	6.43775300

C	1.33438000	-1.95459100	6.09454500
H	0.59884000	-1.79415100	6.87910700
C	3.23642900	-2.33135000	4.06771800
H	3.98588200	-2.49396700	3.30220800
N	0.30375600	-1.91178300	0.14668500
S	-0.69544300	-2.14512500	1.35609200
O	-2.09344200	-2.06825800	0.85900300
O	-0.39567500	-1.43359400	2.60759300
C	-0.45219300	-3.95237100	1.75919800
F	-0.69266700	-4.73103500	0.69428200
F	-1.29147400	-4.30169100	2.73986600
F	0.80392200	-4.15924700	2.16432000
C	0.42949700	3.84800800	-1.12495000
C	0.52915900	3.79822700	0.42931400
H	0.93625500	4.75700300	0.77523000
H	1.23988400	3.01562400	0.69909100
C	-0.73068400	3.54532300	1.19409900
C	-0.26704400	2.52358500	-1.62638400
H	-0.92904200	2.73992100	-2.46591000
H	0.50414000	1.82741800	-1.95980700
N	-1.03792600	1.76479600	-0.61941400
C	-2.37808600	1.60210700	-0.60413700
N	-2.88081800	0.46297800	-0.09609500
C	-4.25743400	0.17901000	0.15882900
C	-5.03622500	0.98645100	0.99152700
C	-4.79557200	-0.98052200	-0.39629200
C	-6.36451900	0.64688900	1.23255400
C	-6.12883100	-1.31279500	-0.14099800
H	-4.17634600	-1.61945500	-1.01664600
C	-6.92179100	-0.50268400	0.66630400
H	-7.95397000	-0.76574200	0.86279200
C	-6.68937100	-2.56199900	-0.77105500
C	-7.22682700	1.55130700	2.07337000
F	-6.02294100	-3.66588000	-0.37027500
F	-7.99245700	-2.74323300	-0.47449700
F	-6.58586100	-2.51761500	-2.12265100
F	-7.94204700	2.40692300	1.30772700
F	-8.11335800	0.85064400	2.81179500
F	-6.49052000	2.30359000	2.92205400
S	-3.38564300	2.92904000	-1.08280700
H	-4.61000600	1.86603300	1.45409800
H	-2.27560000	-0.35839700	0.06050200
H	-0.42870900	1.08094500	-0.13318100
C	-1.88785500	4.32056000	1.19841700

H	-1.80014100	5.32317300	0.77301300
H	-2.51831800	3.77308500	0.14430100
C	-0.37753200	5.09094200	-1.64534500
H	-1.43619800	4.95442000	-1.40447500
H	-0.32214200	5.07712900	-2.73953400
C	1.84078700	3.93606800	-1.74148800
C	1.99255500	3.76041900	-3.12733500
C	2.99007700	4.23392300	-0.99769700
C	3.23742000	3.88018700	-3.74279800
H	1.13149800	3.51692100	-3.74402000
C	4.23959800	4.35381900	-1.61058900
H	2.93194200	4.37270700	0.07571400
C	4.37072800	4.18104800	-2.98655200
H	3.31865800	3.73676500	-4.81689300
H	5.11097300	4.58330000	-1.00287100
H	5.34219000	4.27653200	-3.46400100
C	0.09476600	6.43151900	-1.14942400
C	0.72506600	7.34476000	-1.89396400
H	0.93270400	7.11288800	-2.93981100
H	-0.10666400	6.67224100	-0.10294500
H	-0.70813200	2.68121900	1.85788900
C	1.18730000	8.68890900	-1.41166000
H	2.27375100	8.79790800	-1.52960800
H	0.72662500	9.49971100	-1.99197000
H	0.94274300	8.84661600	-0.35557000
C	-2.90016000	4.19217300	2.33071800
H	-3.91167800	4.44127600	1.99407200
H	-2.91365500	3.17520900	2.73708500
H	-2.64538200	4.87316200	3.15071100

TS-EF-4RR

l imaginary frequency

H = -5315.355867

G = -5315.556113

E(M06-2X-DCM) = -5316.232829

E(M06-2X-cyclohexane) = -5316.204378

O	1.03361000	-2.84185100	0.19703800
O	2.79795600	-1.01822000	-0.28009600
P	1.19392200	-1.23605700	-0.09603900
O	0.74961400	-0.39051700	1.05618400
C	3.02286600	-4.39902500	3.53697300
C	3.67254200	-4.28289700	2.31256300
C	2.98887600	-3.81679400	1.17929200
C	0.98121800	-3.49934500	2.53353400

C	1. 68171300	-4. 02832000	3. 63057700
C	3. 46058100	-1. 63348300	-1. 34428500
C	3. 81618200	-2. 97717600	-1. 25042300
C	4. 30283600	-3. 63219100	-2. 39294200
C	4. 55556000	-2. 92377200	-3. 56300500
C	4. 32295800	-1. 54754300	-3. 58783000
C	3. 75765600	-0. 87420700	-2. 49304100
H	1. 15928900	-4. 12273200	4. 57819000
H	4. 55763400	-0. 97505700	-4. 48041400
C	3. 88066900	-3. 92430300	-0. 05391900
C	5. 29303000	-3. 85208100	0. 62470700
H	5. 54472500	-2. 79962000	0. 79895400
H	6. 07977500	-4. 28345200	-0. 00168500
H	5. 52742600	-5. 38992400	-2. 03493400
H	4. 04964800	-5. 73176000	-2. 92735800
C	1. 66970400	-3. 38700800	1. 31069200
H	3. 55008400	-4. 76657200	4. 41375400
H	4. 94126300	-3. 42763000	-4. 44583400
C	5. 11874200	-4. 57281000	1. 97784400
H	5. 81040800	-4. 20730000	2. 74531900
H	5. 29601100	-5. 65345900	1. 88164100
C	4. 46748200	-5. 11355000	-2. 12444600
C	3. 72148000	-5. 29887700	-0. 78320700
H	2. 65642900	-5. 47593000	-0. 97196600
H	4. 10027500	-6. 13534400	-0. 18713500
C	3. 53035300	0. 60329000	-2. 54869900
C	2. 61321600	1. 15431700	-3. 47705900
C	4. 28419300	1. 45531800	-1. 70152700
C	1. 80776100	0. 35079500	-4. 34720800
C	2. 44977900	2. 58938300	-3. 55099000
C	4. 08346300	2. 88494600	-1. 76384700
C	0. 94480200	0. 91863700	-5. 24674900
H	1. 86165500	-0. 72750000	-4. 26259000
C	1. 54019300	3. 14136500	-4. 50723400
C	3. 17375600	3. 41232800	-2. 68458500
C	0. 81480200	2. 33328400	-5. 33999400
H	0. 33457500	0. 28215200	-5. 88107000
H	1. 44313100	4. 22380200	-4. 55719600
H	3. 02219400	4. 48865400	-2. 72192900
H	0. 12948600	2. 76462400	-6. 06529700
C	-0. 44798200	-3. 09177100	2. 71159800
C	-0. 76392400	-1. 99180600	3. 54575100
C	-1. 48226500	-3. 85123900	2. 11291200
C	0. 23749600	-1. 15296700	4. 13497900

C	-2.14772800	-1.66868400	3.81034500
C	-2.86207100	-3.50905300	2.37330800
C	-0.09724800	-0.09547500	4.94055100
H	1.27887200	-1.35306300	3.91449800
C	-2.45457000	-0.56481300	4.66849200
C	-3.15660600	-2.43764200	3.22216400
C	-1.46282600	0.20019000	5.22055500
H	0.68549200	0.53262200	5.35774400
H	-3.50090300	-0.34668900	4.87206600
H	-4.19789000	-2.20328500	3.43818600
H	-1.71082600	1.03745500	5.86743800
C	5.96814700	1.81767300	0.03535300
H	6.70467700	1.41683700	0.72649800
C	5.26785300	0.96889900	-0.78080700
H	5.46321400	-0.09630100	-0.73667300
C	5.74253400	3.22231300	-0.00997200
H	6.30262400	3.87865900	0.65069800
C	4.82978800	3.73739800	-0.88984500
H	4.64564400	4.80688300	-0.93909300
C	-2.24921200	-5.69440200	0.70334500
H	-2.02480900	-6.54112400	0.06031000
C	-3.60649900	-5.34538400	0.95385200
H	-4.40494900	-5.92638400	0.50021500
C	-3.89979600	-4.28638300	1.76983500
H	-4.93277200	-4.01630300	1.97722300
C	-1.22669500	-4.97717000	1.26660500
H	-0.19934100	-5.26219000	1.07171400
N	0.54738700	-1.02065700	-1.56649900
S	-0.97721200	-1.16301300	-1.91078800
O	-1.41843800	-0.19228000	-2.92653700
O	-1.87762600	-1.31030300	-0.72733300
C	-1.11314200	-2.81450700	-2.77640900
F	-0.32976900	-2.82771100	-3.86063400
F	-2.38414700	-3.01209800	-3.16669900
F	-0.75324600	-3.80960800	-1.96501400
C	-5.08726500	0.50380200	-0.22487500
C	-4.39936600	0.75004700	-1.59901100
H	-5.15725300	0.70210600	-2.39421500
H	-3.72904900	-0.08627500	-1.79529600
C	-3.61609700	1.99821500	-1.79078600
C	-4.09285100	0.90126300	0.93178200
H	-4.42640000	1.81257200	1.42427100
H	-4.07022500	0.09833600	1.67772000
N	-2.70618300	1.13168400	0.50997200

C	-1.94694400	2.17636300	0.94344100
N	-0.62076200	1.96836700	0.99176500
C	0.39365400	2.91828900	1.29547600
C	0.49008900	4.15256900	0.64818500
C	1.35402600	2.54520700	2.24028300
C	1.52528500	5.02417700	0.98353600
C	2.38582100	3.42610300	2.56171700
H	1.28327900	1.57424100	2.71608900
C	2.47391400	4.67291700	1.94498200
H	3.26432100	5.36339700	2.21383800
C	3.43317000	3.00963900	3.56189800
C	1.65721000	6.33985700	0.26345100
F	2.92915700	2.16738000	4.49391800
F	4.46753100	2.37258200	2.97362800
F	3.94681700	4.07572700	4.21631000
F	2.12991300	7.30884500	1.07581500
F	2.52113800	6.25959300	-0.78364900
F	0.47936200	6.76426700	-0.24007300
S	-2.69286600	3.69243700	1.29530500
H	-0.23624000	4.43576500	-0.10105600
H	-0.25959100	0.99027400	0.96449900
H	-2.21105900	0.28096300	0.20212600
C	-3.99656800	3.31670400	-1.48738500
H	-5.05734900	3.45694600	-1.26130600
H	-3.52922500	3.43485900	-0.33294700
C	-5.34971900	-1.04437200	-0.12964200
H	-5.81461000	-1.23198200	0.84880700
H	-4.37923800	-1.55298200	-0.12904800
C	-6.42565200	1.23891400	-0.02462100
C	-6.99179300	1.28908400	1.26249500
C	-7.16357100	1.81124600	-1.07106800
C	-8.22347400	1.89763700	1.49643200
H	-6.46637300	0.84210800	2.10227500
C	-8.39929600	2.42342700	-0.84221100
H	-6.78563800	1.78887700	-2.08804900
C	-8.93539200	2.47254600	0.44252900
H	-8.62652400	1.92091200	2.50534900
H	-8.94018500	2.86055100	-1.67738300
H	-9.89504700	2.94916100	0.62133500
C	-6.22095900	-1.61292200	-1.21497300
C	-5.80021100	-2.49196100	-2.13139800
H	-4.75942200	-2.81727000	-2.10895700
H	-2.64452300	1.84846000	-2.26631300
H	-7.26048800	-1.28157200	-1.23374800

C	-3.33909600	4.47434100	-2.24175300
H	-3.40802200	5.40144300	-1.66488400
H	-2.28086000	4.26948900	-2.43517500
H	-3.83356100	4.63653900	-3.20572700
C	-6.65608700	-3.08615700	-3.21265200
H	-6.69735800	-4.18057100	-3.12782600
H	-7.68211200	-2.70419600	-3.17449400
H	-6.24566300	-2.86771100	-4.20778300

TS-EF-4RR-1

l imaginary frequency

H = -5315.352248

G = -5315.553997

E(M06-2X-DCM) = -5316.230949

E(M06-2X-cyclohexane) = -5316.202796

O	1.50113900	-2.77058800	0.00458600
O	2.94455600	-0.63852800	-0.19731800
P	1.39676200	-1.14879300	-0.19975900
O	0.70129700	-0.46934600	0.93987100
C	3.48272400	-4.22889600	3.39074400
C	4.18833100	-3.91572100	2.23351000
C	3.51842200	-3.47717400	1.08118800
C	1.39601000	-3.58708000	2.28741200
C	2.09594300	-4.08090100	3.40098100
C	3.79677500	-1.03661100	-1.22925900
C	4.36791400	-2.30664700	-1.20167600
C	5.04706000	-2.76858900	-2.34051900
C	5.26875100	-1.92562700	-3.42466000
C	4.81142100	-0.60743500	-3.36665900
C	4.05397900	-0.13718500	-2.28245800
H	1.53225800	-4.32655400	4.29639700
H	5.01784100	0.07380200	-4.18700500
C	4.50077600	-3.33391200	-0.07816000
C	5.82946600	-3.09368000	0.72115800
H	5.88889300	-2.03292300	0.99076200
H	6.71984700	-3.33838900	0.13410200
H	6.51492900	-4.33533000	-2.00805600
H	5.18677200	-4.82494000	-3.05367000
C	2.14015600	-3.27811100	1.13285700
H	4.00107000	-4.57588700	4.28108700
H	5.80186400	-2.27925200	-4.30371500
C	5.68223800	-3.94386100	2.00006100
H	6.24917800	-3.53928000	2.84617200
H	6.04081000	-4.97089600	1.84155800

C	5. 43393500	-4. 22329000	-2. 17145900
C	4. 62795500	-4. 64506700	-0. 92100200
H	3. 62456700	-4. 97102000	-1. 21816300
H	5. 09377400	-5. 46084100	-0. 35879000
C	3. 58408500	1. 28300900	-2. 23776800
C	2. 64571400	1. 76289100	-3. 18415500
C	4. 12463100	2. 16131000	-1. 26364900
C	2. 05150000	0. 92751100	-4. 18420500
C	2. 23640300	3. 14968200	-3. 14175700
C	3. 68436500	3. 53685200	-1. 21773600
C	1. 15524800	1. 42789800	-5. 09124100
H	2. 29364500	-0. 12790600	-4. 19540500
C	1. 29918800	3. 63239100	-4. 10899500
C	2. 75305100	3. 99273700	-2. 15484800
C	0. 77853000	2. 80058800	-5. 06343700
H	0. 70653700	0. 76435800	-5. 82448300
H	1. 01676000	4. 68234800	-4. 07022700
H	2. 41815000	5. 02643500	-2. 10863000
H	0. 07144400	3. 18002800	-5. 79683900
C	-0. 08775800	-3. 40893900	2. 37633800
C	-0. 62243400	-2. 42586800	3. 24479500
C	-0. 95226200	-4. 26139400	1. 64804900
C	0. 19802800	-1. 49694700	3. 96427400
C	-2. 05429800	-2. 31940900	3. 40924600
C	-2. 38322500	-4. 13123500	1. 80512600
C	-0. 34744200	-0. 55654100	4. 79954600
H	1. 27130200	-1. 53223200	3. 82227800
C	-2. 58323100	-1. 33392000	4. 30218100
C	-2. 89330200	-3. 17581600	2. 68963000
C	-1. 75861500	-0. 47767800	4. 98069100
H	0. 30087500	0. 14567000	5. 31695300
H	-3. 66262400	-1. 28025800	4. 42792400
H	-3. 97090000	-3. 10604900	2. 83058900
H	-2. 17431100	0. 26791700	5. 65329700
C	5. 60840900	2. 62606400	0. 62481400
H	6. 35846700	2. 28721700	1. 33439800
C	5. 11694700	1. 75662600	-0. 31315400
H	5. 48890600	0. 73903400	-0. 34518900
C	5. 14822200	3. 97178900	0. 68220700
H	5. 54443900	4. 64397800	1. 43853600
C	4. 21716600	4. 41194400	-0. 21888300
H	3. 85508600	5. 43596500	-0. 19128700
C	-1. 33467200	-6. 08781600	0. 07060300
H	-0. 94190000	-6. 84830500	-0. 59878400

C	-2.74354200	-5.94388100	0.21712200
H	-3.41195400	-6.59279300	-0.34240600
C	-3.24925200	-4.99542300	1.06428100
H	-4.32355800	-4.87913000	1.18953000
C	-0.47248400	-5.27956400	0.76361300
H	0.59728000	-5.40673900	0.64426300
N	0.86624200	-0.95993900	-1.71745500
S	-0.54919700	-1.38967600	-2.25100000
O	-1.03278800	-0.49245700	-3.31393400
O	-1.54128300	-1.72412800	-1.18637600
C	-0.26498500	-3.01151100	-3.13843400
F	0.63753200	-2.83983700	-4.11168700
F	-1.41635500	-3.42358700	-3.68530800
F	0.17533100	-3.95015800	-2.29827000
C	-5.05185500	-0.16043700	-0.83375300
C	-4.23901300	0.08371500	-2.14361400
H	-4.92206700	0.03586300	-3.00246400
H	-3.53025100	-0.73724600	-2.26658300
C	-3.47862900	1.36637000	-2.24976700
C	-4.04828300	-0.07562900	0.37459100
H	-4.47434800	0.45157200	1.22337500
H	-3.81783300	-1.09226500	0.70222900
N	-2.72848400	0.52161100	0.09723600
C	-2.24736900	1.65157400	0.67466500
N	-0.92617200	1.69458400	0.90006400
C	-0.14970800	2.78570100	1.37470900
C	-0.22578300	4.06951300	0.82805100
C	0.76845600	2.51009500	2.39267200
C	0.59065300	5.07901600	1.33545900
C	1.58009300	3.53034200	2.88699400
H	0.83434000	1.50423300	2.79186600
C	1.49109300	4.82158700	2.37048300
H	2.10845700	5.61661500	2.77123200
C	2.58590500	3.22000700	3.96570000
C	0.54861600	6.45436900	0.72415000
F	2.13923400	2.25450300	4.80291100
F	3.75607600	2.78540700	3.45301900
F	2.86231900	4.30953500	4.71662800
F	0.71490900	7.41905300	1.65346400
F	1.53813400	6.62850100	-0.19264800
F	-0.61607300	6.69368200	0.08682300
S	-3.33047500	2.96739600	0.95672200
H	-0.91449200	4.28265800	0.02237600
H	-0.39095900	0.79655700	0.86666100

H	-2.04414100	-0.18454700	-0.20849800
C	-3.96319700	2.65510900	-2.02681500
H	-5.04999500	2.75957600	-1.98590000
H	-3.76715000	2.73996300	-0.73353900
C	-5.57264900	-1.64313400	-0.91109000
H	-4.69161600	-2.28789000	-1.04193800
H	-6.18512200	-1.75170900	-1.81347400
C	-6.28737700	0.76547600	-0.73235000
C	-6.67485100	1.43636700	0.43600700
C	-7.14188300	0.88407800	-1.84515800
C	-7.83857700	2.20914700	0.48397200
H	-6.07414300	1.38356400	1.33507300
C	-8.30373200	1.65277200	-1.80393300
H	-6.90857000	0.36294400	-2.76937800
C	-8.65872200	2.32719500	-0.63487900
H	-8.09731300	2.71971700	1.40776600
H	-8.93199100	1.72078800	-2.68824100
H	-9.56172500	2.93012100	-0.59774500
C	-6.36557200	-2.10396500	0.28219300
C	-7.64266800	-2.49451800	0.24550000
H	-8.16981900	-2.47180900	-0.71001900
H	-2.44459300	1.25627300	-2.58049900
H	-5.84204100	-2.12836200	1.23991800
C	-3.20970400	3.85857900	-2.58525600
H	-3.37122400	4.74785900	-1.96752600
H	-2.13280000	3.66525500	-2.63918500
H	-3.55808000	4.08880000	-3.59856300
C	-8.43797700	-2.97282200	1.42560300
H	-8.80928000	-3.99447700	1.26827000
H	-7.84160300	-2.96704400	2.34438200
H	-9.32083700	-2.34036200	1.58944000

TS-EF-4RR-2

l imaginary frequency

H = -5315.346919

G = -5315.548491

E(M06-2X-DCM) = -5316.227191

E(M06-2X-cyclohexane) = -5316.200086

O	-3.03312700	-0.80015400	-0.93680000
O	-2.37998500	-1.38155700	1.50675800
P	-1.96720000	-0.42077600	0.24541900
O	-2.02502500	0.98240800	0.73239200
C	-7.10229000	-0.16926500	-0.19959300
C	-6.47833600	-1.34053700	0.21757000

C	-5.13066700	-1.58147300	-0.08926700
C	-5.00322200	0.58921400	-1.20384900
C	-6.36978300	0.76735500	-0.92880400
C	-2.32801800	-2.76914200	1.39645000
C	-3.35331800	-3.44950700	0.74047200
C	-3.20049600	-4.82006000	0.47452300
C	-2.11270900	-5.52433100	0.97808300
C	-1.17159500	-4.85052100	1.75614500
C	-1.24292200	-3.46364600	1.96945700
H	-6.85290100	1.67219600	-1.28580500
H	-0.34316500	-5.39791000	2.19571100
C	-4.74912600	-3.00425500	0.30510700
C	-5.78737500	-3.25598600	1.45319400
H	-5.39484200	-2.82332100	2.38076900
H	-5.96367200	-4.32097000	1.63171900
H	-5.03450300	-5.94629500	0.18344900
H	-3.97916600	-5.94039100	-1.22541500
C	-4.39564700	-0.59151700	-0.73647100
H	-8.14861400	0.01570700	0.03031500
H	-1.99923600	-6.58776300	0.78313300
C	-7.05337100	-2.48778700	1.01829900
H	-7.65575700	-2.14825000	1.86866200
H	-7.70918700	-3.11530400	0.39833200
C	-4.33490900	-5.32396000	-0.39192000
C	-5.00070900	-4.01286700	-0.86449100
H	-4.48711500	-3.64220900	-1.75890000
H	-6.06313200	-4.12292800	-1.10371600
C	-0.21619300	-2.80617100	2.83769400
C	1.15540500	-2.85218700	2.47983000
C	-0.60438900	-2.24283100	4.08183400
C	1.61792100	-3.37871900	1.22902700
C	2.15274200	-2.34956600	3.39914800
C	0.40198500	-1.70436700	4.96914900
C	2.95604900	-3.46043500	0.94006700
H	0.89012100	-3.69779000	0.49347700
C	3.53828000	-2.45595100	3.05864300
C	1.74957700	-1.77885600	4.60835000
C	3.93577400	-3.01068300	1.87221100
H	3.27320300	-3.86139200	-0.01855500
H	4.27168700	-2.09263700	3.77522500
H	2.50435500	-1.39713200	5.29330400
H	4.99260000	-3.08903900	1.63171100
C	-4.27365600	1.62298300	-2.00296800
C	-4.09997900	2.92792200	-1.47984000

C	-3.83936000	1.31976900	-3.31741700
C	-4.49326900	3.29135800	-0.15080500
C	-3.49599800	3.95291500	-2.30187300
C	-3.20821000	2.34621200	-4.11545800
C	-4.34747700	4.57292500	0.31323100
H	-4.89948600	2.52619000	0.49973600
C	-3.36183800	5.27874800	-1.77968900
C	-3.06010300	3.63255300	-3.59015800
C	-3.78345200	5.58706800	-0.51334500
H	-4.65524500	4.81840100	1.32599600
H	-2.92671000	6.04190800	-2.42169200
H	-2.60414200	4.40678100	-4.20470200
H	-3.68825500	6.60102100	-0.13330100
C	-2.30387200	-1.66171100	5.74379700
H	-3.34421500	-1.65379200	6.05770800
C	-1.96281400	-2.21016900	4.53520000
H	-2.73541500	-2.63826100	3.90813400
C	-1.31004800	-1.10783900	6.59959300
H	-1.59848300	-0.67970000	7.55583300
C	0.00476300	-1.13485700	6.21991400
H	0.77921100	-0.73467800	6.87037300
C	-3.59163400	-0.22542500	-5.19407300
H	-3.73944900	-1.21311900	-5.62221700
C	-2.94944300	0.78316700	-5.96613300
H	-2.60989300	0.55638500	-6.97309900
C	-2.76911700	2.03272800	-5.43952000
H	-2.28992100	2.81687800	-6.02121500
C	-4.02329600	0.03476500	-3.92045700
H	-4.51669900	-0.74522400	-3.35293200
N	-0.53923600	-0.97739500	-0.32686400
S	-0.09019900	-1.12952100	-1.84006000
O	1.35008700	-1.50291900	-1.82890100
O	-0.48656500	-0.04356000	-2.75014900
C	-0.86623000	-2.69764700	-2.54113300
F	-0.82951200	-3.67414000	-1.62398900
F	-0.15826500	-3.07827100	-3.60816000
F	-2.13373700	-2.50813300	-2.91599600
C	0.30570200	3.62260000	1.17944600
C	-0.14565200	3.44346500	-0.30646000
H	-0.66988900	4.35041600	-0.63646100
H	-0.89066400	2.64498600	-0.32419600
C	0.91901400	3.13268400	-1.30869300
C	0.94627000	2.26494200	1.64370700
H	1.73935000	2.41933800	2.37077000

H	0.16037500	1.68528700	2.12816800
N	1.47238100	1.35618100	0.59748200
C	2.77548700	1.14703200	0.30963500
N	3.09603200	-0.01285300	-0.29176200
C	4.37746100	-0.41105600	-0.75701400
C	4.48780200	-0.91109400	-2.05831300
C	5.48830100	-0.40459400	0.08854600
C	5.72141500	-1.37920000	-2.51266800
C	6.71118200	-0.88508100	-0.37748700
H	5.39151700	-0.05957400	1.11012600
C	6.83978100	-1.36868900	-1.67921200
H	7.79181800	-1.74573500	-2.03248300
C	7.86187300	-0.98837100	0.58757500
C	5.85742300	-1.84684200	-3.93956200
F	7.91002200	0.06709600	1.42736600
F	7.74618100	-2.09797700	1.36066900
F	9.05080600	-1.06765300	-0.04346500
F	6.84532000	-2.75867200	-4.07351500
F	4.71824900	-2.40523100	-4.39463600
F	6.15465000	-0.81852700	-4.76741400
S	3.90879900	2.43291800	0.53485900
H	3.60994100	-0.95326900	-2.69355800
H	2.33128900	-0.63276200	-0.60771500
H	0.82628800	0.59341800	0.35650600
C	2.10716000	3.82832300	-1.51423600
H	2.15527500	4.83445500	-1.09173600
H	2.84211500	3.27597200	-0.55139000
C	-1.01564400	3.81750300	2.01558700
H	-1.69940500	3.00615700	1.75217200
H	-1.47495800	4.75623400	1.67828900
C	1.16727900	4.88562000	1.41089000
C	2.21450700	4.94931600	2.34249400
C	0.81704800	6.08944900	0.76968000
C	2.90027900	6.14057600	2.59424400
H	2.52169500	4.06732200	2.89029800
C	1.49959000	7.28076800	1.01381200
H	-0.01181200	6.11018000	0.06820200
C	2.55381600	7.31311800	1.92718300
H	3.71077200	6.14277400	3.31830800
H	1.19996400	8.18541900	0.49093600
H	3.08964300	8.23834600	2.12015200
C	-0.82490000	3.85473400	3.50757000
C	-1.34813200	2.95464300	4.34785300
H	-1.93984900	2.13531400	3.93593900

H	-0.23471600	4.67775900	3.91339800
H	0.72599900	2.26817000	-1.94770900
C	2.92736200	3.60475500	-2.77829900
H	3.98674500	3.81587100	-2.60263800
H	2.58248700	4.26697400	-3.58071700
H	2.84021400	2.57228200	-3.13226700
C	-1.19715600	2.97462200	5.84167800
H	-2.17324100	3.07230400	6.33703200
H	-0.75798900	2.03569300	6.20377600
H	-0.56463700	3.80506700	6.17448800

TS-EF-4RR-3

l imaginary frequency

H = -5315.343308

G = -5315.545961

E(M06-2X-DCM) = -5316.226524

E(M06-2X-cyclohexane) = -5316.197701

O	-3.03900300	-1.27254500	-0.51412100
O	-2.34268600	-0.66674900	1.90848300
P	-1.97614000	-0.37050700	0.33831600
O	-2.07826700	1.09989000	0.14813100
C	-7.11287800	-0.44314400	-0.06150000
C	-6.45783200	-1.28817200	0.82861500
C	-5.10781300	-1.61985800	0.63848900
C	-5.04128000	-0.18257500	-1.33709500
C	-6.40888000	0.07735900	-1.14780400
C	-2.25689100	-1.95041500	2.43928000
C	-3.27534400	-2.87079000	2.19344000
C	-3.09276700	-4.20810500	2.58206100
C	-1.98285200	-4.58579400	3.32931200
C	-1.04495400	-3.61726800	3.68589200
C	-1.14379300	-2.28973600	3.23627300
H	-6.91539200	0.71798400	-1.86384400
H	-0.19672400	-3.89041000	4.30634400
C	-4.68681600	-2.69823700	1.63126200
C	-5.70739300	-2.41541600	2.78791600
H	-5.31736700	-1.59888900	3.40667200
H	-5.85486600	-3.28349700	3.43742400
H	-4.90272700	-5.37236300	2.87583600
H	-3.86138800	-5.99590800	1.60089600
C	-4.40409200	-1.01847900	-0.40124400
H	-8.16103800	-0.19169700	0.08006400
H	-1.84815100	-5.61775600	3.64343600
C	-6.99659500	-1.95482600	2.07507300

H	-7.60037100	-1.27649000	2.68871500
H	-7.64093200	-2.80876100	1.82232100
C	-4.22365500	-5.07182500	2.06573600
C	-4.92442800	-4.13454900	1.05781200
H	-4.42751600	-4.20575500	0.08355400
H	-5.98593100	-4.36025800	0.91527900
C	-0.10784200	-1.29587400	3.65931000
C	1.25645400	-1.50847200	3.33214200
C	-0.47449800	-0.19929000	4.48404000
C	1.69779600	-2.57143600	2.47673100
C	2.26855300	-0.62546000	3.86970500
C	0.54424000	0.70692300	4.96601900
C	3.03023900	-2.78750000	2.23502300
H	0.95766400	-3.20005500	1.99782600
C	3.64815300	-0.88964900	3.59589400
C	1.88502300	0.46440600	4.65491700
C	4.02561200	-1.95062000	2.81759800
H	3.33086600	-3.59981500	1.57926700
H	4.39324800	-0.22926500	4.03429000
H	2.65056000	1.12936200	5.05068700
H	5.07774800	-2.14192000	2.62421800
C	-4.32985100	0.39995800	-2.51751300
C	-4.15681300	1.80208700	-2.61729300
C	-3.89744100	-0.44761000	-3.56696300
C	-4.55752500	2.71042900	-1.58458200
C	-3.54729300	2.36365800	-3.80213200
C	-3.26386300	0.12580200	-4.73235200
C	-4.41721100	4.06619700	-1.73121600
H	-4.96926000	2.30832500	-0.66682400
C	-3.41066900	3.78355500	-3.91189500
C	-3.11047200	1.51169900	-4.81992700
C	-3.84290700	4.61566900	-2.91394600
H	-4.73822100	4.73021800	-0.93316300
H	-2.96393900	4.18789100	-4.81771700
H	-2.64881100	1.93875700	-5.70838100
H	-3.74836100	5.69375100	-3.01743200
C	-2.14287600	1.11851500	5.69489700
H	-3.17540600	1.27694100	5.99413100
C	-1.82160300	0.04652300	4.90422200
H	-2.60123900	-0.63769800	4.59261800
C	-1.13923100	2.02714100	6.13455000
H	-1.41339800	2.87379100	6.75813400
C	0.16648500	1.81917300	5.78258600
H	0.94881400	2.49156200	6.12753700

C	-3.65357800	-2.65805500	-4.57899800
H	-3.80372500	-3.73330400	-4.53290700
C	-3.00990600	-2.08931300	-5.71405400
H	-2.67114000	-2.73400900	-6.52048500
C	-2.82614100	-0.73574900	-5.78604800
H	-2.34430000	-0.28581800	-6.65104500
C	-4.08347800	-1.86672000	-3.54702100
H	-4.57758500	-2.31891400	-2.69510000
N	-0.53389900	-1.08982300	0.04873400
S	-0.10895500	-1.89852900	-1.25179600
O	1.34573300	-2.18759200	-1.12306100
O	-0.56984300	-1.35802600	-2.53680600
C	-0.83439800	-3.63468500	-1.12970600
F	-0.75844600	-4.07720300	0.13364200
F	-0.12176100	-4.44635000	-1.91586000
F	-2.11019900	-3.67376200	-1.52141600
C	0.36792900	3.70024300	0.30098700
C	-0.13646600	3.27088800	-1.11581900
H	-0.55062700	4.14678100	-1.63083800
H	-0.96523600	2.57666600	-0.96138800
C	0.85863400	2.61964300	-2.02376100
C	0.96465000	2.42948500	1.01390700
H	1.76209900	2.70930900	1.69867900
H	0.16368200	1.97133400	1.59595500
N	1.47399900	1.32366900	0.17329000
C	2.78197000	1.05652600	-0.05479200
N	3.10394100	-0.21498100	-0.34858600
C	4.37754300	-0.72980800	-0.70442100
C	4.44919200	-1.62712900	-1.77593300
C	5.51994400	-0.44343300	0.04522600
C	5.67230100	-2.21150500	-2.10426500
C	6.73270600	-1.04502200	-0.28953600
H	5.45812400	0.21388700	0.90251300
C	6.82165700	-1.92537400	-1.36649900
H	7.76603000	-2.39311900	-1.61657700
C	7.91854800	-0.81133900	0.60800400
C	5.76462800	-3.11792300	-3.30554800
F	8.01798300	0.48229200	0.98056700
F	7.81171100	-1.53792200	1.74977400
F	9.08069100	-1.16158100	0.02154200
F	6.74568900	-4.03586800	-3.16239600
F	4.61144300	-3.77946900	-3.52541900
F	6.04210300	-2.41681800	-4.42938700
S	3.89684100	2.37067600	-0.16016300

H	3.54931800	-1.88054900	-2.32543600
H	2.34199300	-0.91171900	-0.42981900
H	0.83227800	0.51839200	0.13154700
C	2.06364800	3.15287000	-2.47680600
H	2.17727600	4.23523100	-2.38504700
H	2.81750400	2.89889300	-1.42067500
C	-0.89539900	4.09700000	1.16199900
H	-0.55350100	4.25987900	2.19228700
H	-1.56153600	3.22542800	1.16883600
C	1.31337200	4.91973100	0.30666600
C	2.11390800	5.20553900	1.42546000
C	1.29944300	5.87893700	-0.71861700
C	2.89565400	6.35822600	1.49545900
H	2.13338600	4.52893300	2.27380600
C	2.08304500	7.03361800	-0.65904900
H	0.65880800	5.74492400	-1.58385800
C	2.89402300	7.27782600	0.44698400
H	3.50794900	6.53432200	2.37597400
H	2.04726100	7.74533700	-1.47985000
H	3.50619700	8.17399900	0.49693000
C	-1.65941800	5.30363900	0.69476800
C	-1.75769900	6.45404900	1.36747200
H	-1.23040400	6.55283700	2.31823700
H	-2.19551200	5.20065300	-0.24955200
H	0.59248400	1.62222600	-2.37819300
C	2.80296900	2.51245300	-3.64450100
H	3.87790300	2.70860800	-3.58409500
H	2.44128200	2.91675300	-4.59688600
H	2.65613600	1.42746300	-3.66201300
C	-2.54629200	7.65285300	0.92477600
H	-3.31567000	7.92031600	1.66198400
H	-1.89951400	8.53395800	0.81392700
H	-3.04466700	7.47596700	-0.03469300

TS-1-1-4SS

1 imaginary frequency

H = -5315.337149

G = -5315.534679

E(M06-2X-DCM) = -5316.214504

C	2.54780900	4.16290000	-0.16067300
C	1.49802600	4.37857200	0.97729700
H	2.01208100	4.82626700	1.83677900
H	0.77946700	5.11554800	0.60517400
C	0.72738300	3.19681400	1.47536200

C	1. 73594700	3. 77024800	-1. 43094300
H	2. 38390400	3. 33630600	-2. 19697100
H	1. 31165000	4. 68339200	-1. 85017600
N	0. 60918300	2. 87641800	-1. 19978300
C	-0. 69373700	3. 20961600	-1. 53054600
N	-1. 50300700	2. 10825100	-1. 52944500
C	-2. 85375000	1. 91431400	-1. 85789900
C	-3. 85615400	2. 89452700	-1. 82456600
C	-3. 20043300	0. 59572800	-2. 19995500
C	-5. 16872400	2. 54342300	-2. 14362900
C	-4. 51386400	0. 26880200	-2. 52073700
H	-2. 43274400	-0. 17143300	-2. 21444000
C	-5. 51430000	1. 24056900	-2. 50289900
H	-6. 53545300	0. 99070000	-2. 76411900
C	-4. 85734100	-1. 16595500	-2. 81237200
C	-6. 26009400	3. 57380700	-2. 01121500
F	-3. 86651900	-1. 80155400	-3. 48119100
F	-5. 98395000	-1. 28605000	-3. 54143200
F	-5. 05528000	-1. 87368200	-1. 66502900
F	-5. 80267000	4. 83054800	-2. 16804500
F	-6. 84248200	3. 51500700	-0. 78472500
F	-7. 24583600	3. 37912800	-2. 91507000
S	-1. 18940300	4. 78868000	-1. 85103800
H	-3. 60865400	3. 91219800	-1. 55994300
C	1. 15354100	2. 17950500	2. 32929500
H	-1. 02362100	1. 22859700	-1. 30751200
H	0. 81470200	1. 87747500	-1. 16283100
H	1. 22254400	1. 02150400	1. 69594200
O	-1. 11535600	-1. 50015200	0. 74712900
O	1. 12123400	-2. 34274200	-0. 32995900
P	0. 35463500	-1. 01972100	0. 23363200
O	0. 11612500	0. 01428000	-0. 81960100
C	-1. 85470200	-4. 85689700	3. 16800000
C	-1. 45072100	-5. 01105000	1. 84816300
C	-1. 29679400	-3. 89598500	1. 00930000
C	-1. 90298700	-2. 42482000	2. 86048800
C	-2. 12394600	-3. 57654500	3. 63903500
C	0. 65288300	-2. 84536200	-1. 56444000
C	-0. 48433900	-3. 64935300	-1. 56708300
C	-1. 08466100	-3. 98891900	-2. 79065300
C	-0. 49270100	-3. 62629200	-3. 99431200
C	0. 71259700	-2. 92891700	-3. 96761600
C	1. 30656900	-2. 50623100	-2. 76474600
H	-2. 50625800	-3. 44387900	4. 64588400

H	1. 20965600	-2. 67387000	-4. 89865700
C	-1. 19174200	-4. 37858100	-0. 43448800
C	-0. 54792300	-5. 78858300	-0. 21569400
H	-0. 71715100	-6. 45884900	-1. 06398800
H	0. 53454800	-5. 66503500	-0. 09600500
H	-3. 19263700	-4. 35156000	-3. 17831700
H	-2. 26277700	-5. 80742000	-2. 82128000
C	-1. 41344400	-2. 61431300	1. 55032700
H	-1. 99230200	-5. 71955200	3. 81476000
H	-0. 95111200	-3. 89142500	-4. 94343700
C	-1. 16518600	-6. 29541100	1. 10283300
H	-2. 08747900	-6. 86527900	0. 92353100
H	-0. 49027700	-6. 95703900	1. 65781300
C	-2. 37463800	-4. 74465600	-2. 56585800
C	-2. 62108000	-4. 54260200	-1. 05636200
H	-3. 18337400	-5. 35865400	-0. 59310300
H	-3. 18816600	-3. 61831200	-0. 90218400
C	2. 61512200	-1. 78605500	-2. 86927200
C	3. 81314600	-2. 45426600	-2. 51402200
C	2. 66746800	-0. 51648900	-3. 49503300
C	3. 83048000	-3. 75632500	-1. 91965400
C	5. 08748100	-1. 83000300	-2. 79151600
C	3. 94898100	0. 08277500	-3. 79305900
C	5. 00765300	-4. 37770700	-1. 59441300
H	2. 88891800	-4. 25554300	-1. 72258500
C	6. 29302700	-2. 51097500	-2. 43336400
C	5. 12113600	-0. 58760600	-3. 43202300
C	6. 25867000	-3. 74730500	-1. 84754900
H	4. 98893000	-5. 36360800	-1. 13822100
H	7. 24164800	-2. 02305200	-2. 64506700
H	6. 08395100	-0. 13793100	-3. 66756200
H	7. 18143000	-4. 25516800	-1. 58091200
C	-2. 28782300	-1. 11209200	3. 46741800
C	-3. 33203800	-0. 33978100	2. 89316600
C	-1. 72254300	-0. 72516000	4. 71173500
C	-4. 00778300	-0. 70646400	1. 68513700
C	-3. 78877300	0. 85757300	3. 56564900
C	-2. 23430500	0. 43957000	5. 39943600
C	-5. 00153300	0. 07315000	1. 15401800
H	-3. 73438000	-1. 62713500	1. 18439100
C	-4. 81216500	1. 65664300	2. 96389600
C	-3. 24154900	1. 20279300	4. 80395400
C	-5. 39765400	1. 28652500	1. 78415100
H	-5. 49203800	-0. 24202900	0. 23981900

H	-5.11711800	2.56760300	3.47382500
H	-3.61152000	2.08768900	5.31844100
H	-6.15735500	1.90951100	1.32086700
C	1.57242000	1.42215000	-4.50833800
H	0.66409200	1.95354900	-4.77875100
C	1.49097900	0.21284200	-3.86710000
H	0.52241500	-0.20491100	-3.62118900
C	2.83900900	1.99610300	-4.82137400
H	2.88392400	2.94984100	-5.34015600
C	3.99056000	1.34530000	-4.46596100
H	4.96348300	1.77452300	-4.69396700
C	-0.12251600	-1.03399600	6.53596500
H	0.71477100	-1.57674200	6.96567600
C	-0.66324500	0.08530900	7.22922100
H	-0.25147500	0.37406100	8.19252800
C	-1.68425300	0.80374300	6.66866300
H	-2.09568000	1.67385800	7.17531500
C	-0.63150600	-1.42577600	5.32414300
H	-0.17881800	-2.25771200	4.79917000
N	1.30361000	-0.42647700	1.44088500
S	2.20511800	-1.28718200	2.50680700
C	3.70871900	-1.87971900	1.51317900
O	1.54522600	-2.51989100	2.94589900
O	2.73931000	-0.33499100	3.48107200
F	3.55657200	-3.16211500	1.18936900
F	3.86164600	-1.15578400	0.40364200
F	4.79586100	-1.74747900	2.27750000
H	-0.34479800	3.23035300	1.27884700
H	2.18607200	2.24464200	2.67462200
C	3.66194100	3.18144400	0.24780300
C	4.24918400	3.26997100	1.52481600
C	4.20030700	2.23651800	-0.63627300
C	5.30942300	2.44894900	1.90434400
H	3.88196700	3.99626600	2.24243400
C	5.26697000	1.41502100	-0.26189100
H	3.79860300	2.11569100	-1.63557300
C	5.82590700	1.51221500	1.00920900
H	5.72540500	2.53962800	2.90405300
H	5.64006000	0.68146600	-0.96940400
H	6.64346000	0.86059200	1.30410300
C	3.18635100	5.56005000	-0.51007200
H	3.79620800	5.40601500	-1.41225000
H	2.36861200	6.23459400	-0.79295900
C	4.02619100	6.22962000	0.54264500

H	4.99049100	5.77540500	0.76672600
C	3.67490200	7.34967800	1.18475900
H	2.71394700	7.81178900	0.94872200
C	0.14167000	1.74513700	3.40469500
H	-0.84231000	1.54486500	2.97243700
H	0.49723200	0.84680000	3.90684800
H	0.03188800	2.53378200	4.15692000
C	4.51079200	8.05718700	2.21251300
H	4.74714000	9.08131700	1.89351000
H	3.97786300	8.14421700	3.16906500
H	5.45482500	7.53300500	2.39537200

TS-1-1-4RS

1 imaginary frequency

H = -5315.338489

G = -5315.538954

E(M06-2X-DCM) = -5316.217345

C	4.50434100	0.90247400	-1.34957700
C	3.63978600	0.87653800	-2.65492600
H	4.19667400	0.27734600	-3.38639600
H	3.56273800	1.90536800	-3.02112200
C	2.25326100	0.32304100	-2.60645100
C	3.79789600	1.82356000	-0.30134600
H	4.16137700	1.57766900	0.70146200
H	4.06334000	2.86066300	-0.50855100
N	2.34037900	1.76980700	-0.29515600
C	1.55003600	2.90890700	-0.44098200
N	0.24157000	2.62917400	-0.19284200
C	-0.88290300	3.46985900	-0.07145400
C	-1.11592000	4.61553300	-0.84088500
C	-1.85739300	3.04707600	0.84431200
C	-2.31329800	5.31594800	-0.68020000
C	-3.03678100	3.76980900	1.00559400
H	-1.67623600	2.15659800	1.43536500
C	-3.27810900	4.91286900	0.24338100
H	-4.19831700	5.47212500	0.35935100
C	-4.01310900	3.33966000	2.06611900
C	-2.61704400	6.45526300	-1.61587400
F	-4.10284000	1.98994300	2.15130900
F	-3.64091300	3.77624400	3.29728900
F	-5.25502500	3.81506900	1.84255300
F	-3.49157900	7.33442100	-1.08053300
F	-1.51039000	7.13920500	-1.96623800
F	-3.17725300	5.99681200	-2.76653300

S	2.15894700	4.40719800	-0.89726700
H	-0.37661600	4.94571600	-1.55705000
C	1.87717500	-1.01878000	-2.68271200
H	-0.01785200	1.63489200	-0.14960900
H	2.70145400	-1.72728600	-2.80016000
H	1.93934800	1.05488600	0.30356200
H	1.43462100	-1.34626100	-1.49767300
O	-1.80816700	-2.18793400	-0.04484600
O	-0.59100200	-0.62688500	1.65301900
P	-0.58955200	-1.13114700	0.09957700
O	-0.69563400	0.10796500	-0.72053500
C	-5.68059600	-0.67397800	0.50348600
C	-4.92089400	-1.08967100	1.59061900
C	-3.65179300	-1.66062900	1.40322200
C	-3.87337400	-1.33186300	-1.00959600
C	-5.16363500	-0.82379600	-0.78205200
C	-0.54320300	-1.44645700	2.79013200
C	-1.63602700	-2.24360800	3.12511300
C	-1.47746500	-3.21465400	4.12727700
C	-0.31320800	-3.27169000	4.88454600
C	0.68832900	-2.33017600	4.65520500
C	0.60724700	-1.40386400	3.60223900
H	-5.75405400	-0.52171400	-1.64180300
H	1.56882600	-2.31193500	5.28998600
C	-3.11133300	-2.18037100	2.72936300
C	-3.87763900	-1.23377800	3.72051900
H	-3.94093300	-1.64965300	4.73017800
H	-3.33844300	-0.28151500	3.78284200
H	-3.26543300	-3.88656300	5.15920800
H	-2.46762200	-5.15136200	4.23123400
C	-3.12628600	-1.72229900	0.11752500
H	-6.66430900	-0.23532300	0.64886200
H	-0.19508500	-4.01481700	5.66887700
C	-5.25077100	-0.99332300	3.06201400
H	-5.67841500	-0.02053000	3.32664800
H	-5.98158400	-1.75841000	3.35906400
C	-2.71312300	-4.08327200	4.23001200
C	-3.52857200	-3.66473200	2.98651100
H	-3.22602500	-4.26800500	2.12280800
H	-4.60936300	-3.77873800	3.11588500
C	1.68099300	-0.36994800	3.46589500
C	3.03083400	-0.75977000	3.26591400
C	1.36288200	0.99818700	3.68424100
C	3.41645800	-2.11517400	3.00198000

C	4. 07973100	0. 23526900	3. 32417300
C	2. 41804900	1. 98735500	3. 68039700
C	4. 73383900	-2. 46387700	2. 84909700
H	2. 64615300	-2. 86959100	2. 89893900
C	5. 44288200	-0. 17568800	3. 17671500
C	3. 74496800	1. 57817200	3. 51929900
C	5. 76533000	-1. 48777800	2. 95255200
H	4. 99365500	-3. 49700200	2. 63718500
H	6. 21912400	0. 58263400	3. 25474900
H	4. 53644500	2. 32440700	3. 55341800
H	6. 80416200	-1. 78759700	2. 84420500
C	-3. 39211000	-1. 45759000	-2. 42089800
C	-3. 18884500	-0. 29233300	-3. 20242900
C	-3. 25490500	-2. 74219000	-3. 00341400
C	-3. 28655700	1. 03453300	-2. 66764800
C	-2. 85753900	-0. 42524100	-4. 60399100
C	-2. 89448800	-2. 85777100	-4. 39869600
C	-3. 10760300	2. 13937600	-3. 45973300
H	-3. 49029400	1. 15822700	-1. 61086500
C	-2. 67980800	0. 75301200	-5. 39546900
C	-2. 71439400	-1. 69956500	-5. 15992900
C	-2. 80755800	1. 99927200	-4. 84517400
H	-3. 18518700	3. 13585000	-3. 03350400
H	-2. 44056800	0. 63248700	-6. 44959800
H	-2. 46312000	-1. 79248600	-6. 21480400
H	-2. 67321300	2. 88681500	-5. 45750200
C	-0. 24165700	2. 79424500	4. 12768000
H	-1. 26503600	3. 11454200	4. 30090100
C	0. 03290200	1. 46305700	3. 94605500
H	-0. 77243200	0. 74111900	4. 01086400
C	0. 79808900	3. 76525800	4. 07576800
H	0. 56114200	4. 81670400	4. 21021100
C	2. 09036000	3. 36706000	3. 86886900
H	2. 89770000	4. 09460000	3. 84203500
C	-3. 34694400	-5. 18177700	-2. 87323100
H	-3. 52947700	-6. 08454900	-2. 29650700
C	-2. 96577200	-5. 28924700	-4. 24073300
H	-2. 85516000	-6. 27059300	-4. 69390400
C	-2. 75126600	-4. 15716600	-4. 97902300
H	-2. 47235000	-4. 22318000	-6. 02812300
C	-3. 48950500	-3. 95514900	-2. 27915500
H	-3. 78864000	-3. 89603400	-1. 23913800
N	0. 74967400	-1. 98942400	-0. 34826700
S	1. 21445300	-3. 50227900	0. 06029400

C	0.10879600	-4.71947300	-0.86572500
O	2.53701600	-3.70611300	-0.53243400
O	0.96636500	-3.81685000	1.46901700
F	0.74199500	-5.89558500	-0.88654400
F	-0.10158100	-4.32000200	-2.12426400
F	-1.06105600	-4.87027800	-0.24663900
C	5.87898200	1.55100200	-1.62363000
C	6.78772500	1.68519700	-0.55781500
C	6.27367400	2.04624800	-2.87390500
C	8.03033700	2.29081600	-0.73386400
H	6.52679500	1.30863800	0.42704200
C	7.52070300	2.65045200	-3.05493100
H	5.61540200	1.96835700	-3.73210400
C	8.40541800	2.77787100	-1.98687200
H	8.70726300	2.37983200	0.11184300
H	7.79436800	3.02221000	-4.03881500
H	9.37432200	3.24896300	-2.12719000
C	4.72403600	-0.54695600	-0.81538200
H	5.23548800	-0.46390000	0.15287500
H	3.76481100	-1.02948700	-0.59781300
C	5.55351900	-1.41580400	-1.73014500
C	5.28016700	-2.67963600	-2.07287100
H	4.38232500	-3.15658800	-1.68365200
H	6.47336700	-0.96256000	-2.10228300
H	1.44313700	1.04828300	-2.66056700
C	0.60950000	-1.34046700	-3.49300700
H	0.24590000	-2.34076000	-3.26042200
H	-0.18672500	-0.62621900	-3.27289400
H	0.83389100	-1.29741100	-4.56469100
C	6.16113300	-3.52975200	-2.94472900
H	7.04285300	-2.98002000	-3.29251200
H	6.50753000	-4.42103600	-2.40394400
H	5.61720400	-3.89589700	-3.82621800

TS-1-1-4SR

1 imaginary frequency

H = -5315.339219

G = -5315.541071

E(M06-2X-DCM) = -5316.219950

C	3.66226700	2.06163500	2.02032800
C	2.69588100	1.91661200	3.26710400
H	3.24916400	1.38094500	4.04382000
H	2.49050200	2.93178800	3.62479900
C	1.39422600	1.22279700	3.07380300

C	2.96683700	2.99305700	0.99952000
H	3.54015400	3.02052400	0.06471300
H	2.91775400	4.00711200	1.39575700
N	1.59071400	2.61657300	0.70052300
C	0.54483200	3.52521300	0.70287700
N	-0.56035800	3.00265800	0.09014500
C	-1.81783100	3.52775500	-0.24474800
C	-2.22264500	4.86197800	-0.10297100
C	-2.71198100	2.60025400	-0.81470600
C	-3.49920700	5.24155100	-0.52682200
C	-3.97292000	3.00271300	-1.23529400
H	-2.41166300	1.56290600	-0.91902100
C	-4.38532400	4.33017500	-1.09467900
H	-5.37043000	4.64340600	-1.41864200
C	-4.88956300	2.00973600	-1.89622400
C	-3.94158700	6.66582200	-0.30390600
F	-4.58792600	0.73257300	-1.55367600
F	-4.82571300	2.07187100	-3.24712200
F	-6.18213900	2.21701500	-1.55561900
F	-4.90440900	7.03439600	-1.17909900
F	-2.91941200	7.53707700	-0.43405700
F	-4.45164600	6.83737100	0.93723900
S	0.64706800	5.03353800	1.44510200
H	-1.54999800	5.58888000	0.32855400
C	1.16841500	-0.14702800	3.24149100
H	-0.47144700	2.01435900	-0.16770900
H	1.46112700	1.80906100	0.09346100
H	1.04710100	-0.66637100	2.08649900
O	-1.75858600	-1.43507900	-0.00613900
O	0.24862100	-1.97277200	-1.59972500
P	-0.17198700	-1.14682400	-0.26090100
O	-0.02338000	0.33342600	-0.40188900
C	-3.53721000	-5.24518400	-0.10636300
C	-3.08441000	-4.64492300	-1.27414200
C	-2.58538600	-3.33322900	-1.26022900
C	-2.94353400	-3.22445200	1.14996200
C	-3.51071700	-4.51104500	1.07398800
C	-0.23754000	-1.45920700	-2.82120000
C	-1.54419600	-1.75708900	-3.19846800
C	-2.11294300	-1.09323700	-4.29681000
C	-1.34718600	-0.23707200	-5.07936100
C	-0.00213300	-0.06080100	-4.76388300
C	0.58320900	-0.64776500	-3.62707800
H	-3.92702000	-4.93686700	1.98115200

H	0.62278800	0.56441900	-5.39426500
C	-2.49926600	-2.82674800	-2.69613100
C	-2.25585500	-4.17134200	-3.45884600
H	-2.52885400	-4.10269700	-4.51650800
H	-1.19008600	-4.42074300	-3.40195100
H	-4.20418200	-0.56509800	-4.56291700
H	-3.74047300	-2.08347400	-5.33210600
C	-2.40853100	-2.68138100	-0.03771300
H	-3.93896300	-6.25507800	-0.11575800
H	-1.78025200	0.27369700	-5.93548600
C	-3.07919800	-5.21353200	-2.67555600
H	-4.09984600	-5.30288700	-3.07272500
H	-2.63809800	-6.21608500	-2.71533600
C	-3.57363300	-1.45426800	-4.44702400
C	-3.87270700	-2.21349300	-3.13641200
H	-4.64988100	-2.97585800	-3.24376600
H	-4.20574000	-1.50380700	-2.37403900
C	2.04568300	-0.42291200	-3.41090000
C	2.95640100	-1.49203900	-3.60409500
C	2.52758400	0.89131200	-3.19193300
C	2.53773400	-2.83335100	-3.88006800
C	4.37792500	-1.23181400	-3.56920400
C	3.95093000	1.14239700	-3.20159000
C	3.44647200	-3.84191900	-4.06483200
H	1.47801800	-3.05072400	-3.94340200
C	5.29316400	-2.31383800	-3.76120100
C	4.83451500	0.07583400	-3.38485100
C	4.84500700	-3.58499000	-3.99674600
H	3.09801400	-4.85095800	-4.26735400
H	6.35838500	-2.09837800	-3.72290400
H	5.90504500	0.26879400	-3.39480900
H	5.54997500	-4.39890100	-4.14204000
C	-3.04987400	-2.52312200	2.46875800
C	-3.85227800	-1.35773100	2.59482400
C	-2.50181200	-3.13520900	3.62738700
C	-4.49162900	-0.71761800	1.48406700
C	-4.09330900	-0.79685200	3.90707400
C	-2.78220500	-2.58004200	4.93327200
C	-5.27343400	0.39653400	1.64881400
H	-4.36169200	-1.12933000	0.49119000
C	-4.90332000	0.37508300	4.03442500
C	-3.56185900	-1.42585500	5.03569100
C	-5.47731100	0.96023300	2.93950400
H	-5.74814300	0.85270000	0.78625700

H	-5.06063800	0.78361200	5.02998400
H	-3.76915700	-1.01079100	6.02023900
H	-6.09508200	1.84730200	3.04902500
C	2.15239100	3.27833700	-2.80478400
H	1.47010500	4.10688200	-2.63631300
C	1.65835700	2.00925700	-2.96812400
H	0.58977300	1.83579000	-2.92063000
C	3.55536300	3.52408400	-2.84816200
H	3.92770800	4.53819200	-2.73138100
C	4.42512000	2.48225700	-3.03412700
H	5.49853300	2.65530800	-3.06531100
C	-1.14668700	-4.85972200	4.71007700
H	-0.48722600	-5.71909600	4.63065100
C	-1.45880100	-4.33023600	5.99355900
H	-1.05618600	-4.80373600	6.88495700
C	-2.24848400	-3.21736800	6.09706000
H	-2.48334800	-2.79005800	7.06929400
C	-1.64914700	-4.28643800	3.57052100
H	-1.37104600	-4.68952500	2.60426600
N	0.78225600	-1.69100600	0.96605600
S	1.25125100	-3.21747300	1.29855700
C	2.93984600	-3.33922300	0.49818700
O	0.42585700	-4.22783200	0.63160700
O	1.53447700	-3.30535400	2.73306900
F	2.87864600	-3.04861700	-0.79887400
F	3.78535900	-2.48955300	1.09941500
F	3.39738600	-4.58421600	0.65429100
H	0.52271400	1.85145500	2.90104100
H	2.02634700	-0.71471900	3.61322600
C	-0.17573600	-0.58241900	3.84451200
H	-1.01999500	-0.09413500	3.34895000
H	-0.28293600	-1.66016300	3.73973200
H	-0.20792500	-0.33380200	4.91043700
C	4.97314300	2.68351400	2.54224200
C	5.73771200	1.98766300	3.49469600
C	5.45971900	3.92300800	2.10441700
C	6.92574700	2.50994700	3.99900900
H	5.40961000	1.01323900	3.84683400
C	6.65419700	4.44955600	2.60493800
H	4.92115200	4.50028900	1.36193200
C	7.39123000	3.74992400	3.55646300
H	7.48991300	1.94522000	4.73653600
H	7.00178100	5.41426400	2.24501700
H	8.31738600	4.16147100	3.94805200

C	3.94484700	0.65375100	1.40551900
H	4.12885000	-0.06533700	2.21128200
H	3.03277500	0.30454400	0.90158000
C	5.10479300	0.60964500	0.44636400
H	5.08034100	1.30717600	-0.39059000
C	6.13441800	-0.23386100	0.55489000
H	6.14924700	-0.94004400	1.38673000
C	7.29980200	-0.30973500	-0.38799300
H	8.24951700	-0.16466300	0.14425000
H	7.35629000	-1.29472000	-0.87136300
H	7.23315500	0.45080900	-1.17287300

TS-1-2-4SS

l imaginary frequency

H = -5315.334952

G = -5315.538852

E(M06-2X-DCM) = -5316.222705

O	-1.90025900	1.17874900	1.42163000
O	-2.90350600	-1.15330400	0.81250900
P	-1.72318800	-0.10232200	0.42272400
O	-1.89687100	0.46420200	-0.97325000
N	-0.30639700	-0.77822900	0.78459800
S	0.09413100	-2.31761900	0.66126600
C	-0.20948500	-3.02572300	2.36916800
F	0.05557500	-4.33336300	2.35494600
F	0.58273200	-2.43613100	3.27490100
F	-1.48444100	-2.84148100	2.73269500
C	0.78361400	2.89729300	-2.91056900
C	0.98700300	1.66113200	-3.87035600
H	0.43967400	1.86940500	-4.79613500
H	2.05402000	1.61377500	-4.09954800
C	0.56580100	0.32004300	-3.38052100
C	1.53392000	2.62058700	-1.56088500
H	0.98237400	3.02554100	-0.71504100
H	2.48680200	3.14750100	-1.59298900
N	1.83355000	1.21676400	-1.24959400
C	3.11064300	0.69739400	-1.40061400
N	3.29001700	-0.49198200	-0.76178100
C	4.49113900	-1.23704300	-0.64712300
C	5.71546800	-0.62885400	-0.35703200
C	4.41635700	-2.63224000	-0.73589800
C	6.85000900	-1.41508600	-0.15906900
C	5.56262100	-3.40391300	-0.54533000
H	3.46180000	-3.10920200	-0.92353900

C	6. 78851300	-2. 80406400	-0. 25599600
H	7. 67360500	-3. 40744300	-0. 09698800
C	5. 48893100	-4. 89889200	-0. 71457700
C	8. 12436600	-0. 72724000	0. 24964900
F	4. 27400200	-5. 38555200	-0. 38926900
F	6. 40353800	-5. 53450100	0. 05221700
F	5. 73099500	-5. 26486300	-1. 99583400
F	9. 18989400	-1. 55349200	0. 21373900
F	8. 03569300	-0. 24925100	1. 52030500
F	8. 40040900	0. 33260600	-0. 53854600
S	4. 27660500	1. 43519400	-2. 37225200
C	1. 52148700	4. 09174400	-3. 61599700
H	2. 56291600	3. 79388100	-3. 78310700
H	1. 06545700	4. 23742500	-4. 60488400
H	5. 77576000	0. 44659000	-0. 26791500
C	-0. 73336300	-0. 18114100	-3. 27451000
H	2. 49391100	-0. 94285000	-0. 29754900
H	-1. 50848400	0. 40524200	-3. 77892100
O	1. 56376900	-2. 39377000	0. 51345900
H	1. 27981200	0. 80596100	-0. 49819700
O	-0. 73512200	-3. 12435400	-0. 23961400
H	-1. 06593200	0. 16223600	-2. 10684700
C	-6. 88274600	0. 17120500	0. 68445300
C	-6. 08459600	0. 41785200	1. 79587000
C	-4. 77535000	-0. 08171400	1. 86044000
C	-5. 04415100	-1. 07356800	-0. 35372700
C	-6. 36683800	-0. 59379000	-0. 35902900
C	-1. 71409200	0. 99314700	2. 80118700
C	-2. 72049100	0. 38663200	3. 55109200
C	-2. 45317700	0. 00411300	4. 87522000
C	-1. 25101800	0. 34842200	5. 48207800
C	-0. 32278900	1. 09758400	4. 76127500
C	-0. 51880100	1. 42695100	3. 40819900
H	-6. 99132900	-0. 82962000	-1. 21534800
H	0. 59392300	1. 42637700	5. 24090500
C	-4. 19704000	0. 15174200	3. 24978600
C	-5. 03794000	1. 39863800	3. 69537900
H	-5. 07562900	1. 50934200	4. 78313000
H	-4. 56973900	2. 30122800	3. 28546300
H	-3. 29681400	-1. 68963700	5. 95660600
H	-4. 16300600	-0. 17694000	6. 19900300
C	-4. 24726700	-0. 75861400	0. 76264500
H	-7. 89949500	0. 55222400	0. 63239200
H	-1. 04252100	0. 06260300	6. 50984600

C	-6.42273700	1.19444500	3.04835000
H	-7.08992300	0.61659900	3.70333200
H	-6.93450200	2.13972000	2.83438800
C	-3.61807100	-0.77115400	5.45242900
C	-4.48708700	-1.05119100	4.20644000
H	-5.55252300	-1.15910200	4.43231000
H	-4.14911600	-1.97361800	3.72081200
C	0.50224600	2.28972000	2.73595000
C	0.15649600	3.61315700	2.35423300
C	1.84687600	1.85067000	2.63317900
C	-1.16846800	4.14503300	2.47968200
C	1.18156500	4.50156600	1.85166700
C	2.86678600	2.76469000	2.16803000
C	-1.46516800	5.42934100	2.10234500
H	-1.94849000	3.51837500	2.89530700
C	0.82798300	5.83183400	1.46171500
C	2.50568300	4.05794500	1.78206900
C	-0.45756600	6.28612300	1.57594600
H	-2.47935500	5.80340700	2.21509200
H	1.61279800	6.47868600	1.07813400
H	3.27544600	4.73988000	1.42689900
H	-0.71214100	7.29982600	1.27920400
C	-4.61807000	-1.94182600	-1.49580700
C	-4.41192700	-3.32877100	-1.28761400
C	-4.58264500	-1.40520200	-2.80700800
C	-4.45030900	-3.93885700	0.00701000
C	-4.18612700	-4.19295400	-2.42498000
C	-4.39376100	-2.28799700	-3.93627500
C	-4.24907600	-5.28405900	0.16875400
H	-4.64223900	-3.31963200	0.87514400
C	-3.97754600	-5.59154400	-2.21178200
C	-4.20224800	-3.65417200	-3.71429300
C	-4.00253700	-6.12536500	-0.95275300
H	-4.27623100	-5.71714700	1.16493200
H	-3.79950200	-6.22230800	-3.07945900
H	-4.05753400	-4.31537400	-4.56645100
H	-3.83949900	-7.18899100	-0.80278300
C	3.57274600	0.14277300	2.91248700
H	3.85011200	-0.87554000	3.16945000
C	2.25663800	0.52079600	2.97503200
H	1.50417400	-0.19854400	3.26923400
C	4.58013200	1.06080300	2.49733900
H	5.61757600	0.74109600	2.45692100
C	4.22942400	2.32985900	2.12227000

H	4.98248200	3.03655400	1.78217000
C	-4.68373700	0.48322300	-4.35666800
H	-4.76300000	1.55324900	-4.52576500
C	-4.53934000	-0.39668200	-5.46779700
H	-4.53600900	0.00555700	-6.47746700
C	-4.39232900	-1.74156100	-5.25821200
H	-4.26536300	-2.42366900	-6.09583200
C	-4.70557200	-0.00273400	-3.07439800
H	-4.78701200	0.68421300	-2.24025900
C	-0.71272700	3.26343500	-2.78154900
C	-1.45154300	3.52679400	-3.95259900
C	-1.37721400	3.43489400	-1.56089400
C	-2.78028800	3.94147200	-3.90660400
H	-0.98301100	3.42382000	-4.92790600
C	-2.71104600	3.84974300	-1.50808000
H	-0.88376100	3.23939800	-0.61789400
C	-3.42054300	4.10930200	-2.67642200
H	-3.31088400	4.14308900	-4.83381500
H	-3.18418400	3.96356200	-0.53728400
H	-4.45534400	4.43858500	-2.63404800
C	1.48652000	5.39356400	-2.86229700
C	2.57585100	6.07821400	-2.49845000
H	3.55873400	5.66642300	-2.73507300
H	1.37104100	-0.37755000	-3.15635600
H	0.50102600	5.79890800	-2.63098400
C	-0.93385200	-1.69824600	-3.28354100
H	-1.05582600	-2.05193900	-4.31326900
H	-0.08095300	-2.21628700	-2.83546400
H	-1.82115200	-1.98303100	-2.71947500
C	2.56872000	7.40622600	-1.79702700
H	3.04746000	8.18134300	-2.41109300
H	1.54971900	7.73663700	-1.56905200
H	3.13490600	7.36456500	-0.85637200

TS-1-2-4SR

1 imaginary frequency

H = -5315.334738

G = -5315.536995

E(M06-2X-DCM) = -5316.226482

O	-0.81701600	-0.25782900	1.88139200
O	-2.37641600	-1.78576300	0.44777400
P	-1.03805800	-0.86819600	0.38676000
O	-1.24034600	0.40562000	-0.43607100
N	0.21256400	-1.80718100	0.06145100

S	0.28298600	-2.91794100	-1.10125200
C	-0.05739500	-4.51868000	-0.18753300
F	-0.13450100	-5.51746900	-1.07083300
F	0.93011200	-4.78614800	0.67884400
F	-1.20955400	-4.44896900	0.49066100
C	-1.28592500	4.19562200	-0.84427500
C	-1.44938100	3.63578100	-2.32153900
H	-2.50916800	3.43620600	-2.50185600
H	-1.13760600	4.43973400	-3.00281100
C	-0.64756200	2.45231900	-2.74263900
C	0.17636300	4.04835000	-0.36306900
H	0.24409400	4.36285000	0.68458800
H	0.83084500	4.69498800	-0.94808700
N	0.73543200	2.70369100	-0.48394100
C	1.98508900	2.45948100	-1.00303700
N	2.43727200	1.18553700	-0.79326800
C	3.70530100	0.66331700	-1.17707700
C	4.88267800	1.36792800	-0.91108800
C	3.76661400	-0.60504500	-1.75788100
C	6.11234600	0.80709700	-1.24553900
C	5.00918700	-1.15183600	-2.09061400
H	2.86294000	-1.18024600	-1.93193100
C	6.18706300	-0.45008300	-1.84634800
H	7.14641200	-0.87630100	-2.11212600
C	5.07718000	-2.54512900	-2.66324700
C	7.36493300	1.53163800	-0.83845100
F	4.05310400	-2.79971200	-3.49730800
F	5.04765600	-3.48402500	-1.68948600
F	6.22560800	-2.73962500	-3.35664000
F	7.27365400	2.86231500	-1.03696200
F	8.45403700	1.08999100	-1.49955600
F	7.61588000	1.35919500	0.49176400
S	2.81984700	3.60145200	-1.92645600
H	4.83763200	2.33931000	-0.43838300
C	-1.14675700	1.18097200	-3.00060400
H	1.81297600	0.50978600	-0.35827200
H	-2.23448800	1.10733400	-3.08188300
O	1.66593200	-3.05604500	-1.56716900
H	0.30722400	1.97763000	0.08496000
O	-0.79703500	-2.81188300	-2.09552100
H	-1.08449900	0.81158300	-1.76262500
C	-6.07813300	-0.15722400	1.55455500
C	-5.11345800	-0.44399600	2.51362500
C	-3.91184600	-1.07357100	2.15225500

C	-4.60043000	-1.03608300	-0.19218800
C	-5.83081300	-0.49631600	0.22569700
C	-0.59997300	-1.11563300	2.97109500
C	-1.68875900	-1.76556900	3.55214800
C	-1.45344200	-2.74341400	4.53283200
C	-0.16924600	-2.97927100	5.00866100
C	0.88604600	-2.22456500	4.50284400
C	0.70572200	-1.28900100	3.46850800
H	-6.59739800	-0.32672200	-0.52408800
H	1.88885900	-2.36816700	4.89277400
C	-3.19310800	-1.54741900	3.41109800
C	-3.70309300	-0.47926600	4.43634600
H	-3.61634100	-0.81972200	5.47242900
H	-3.09621400	0.42735500	4.33026800
H	-2.63933500	-4.51828100	4.97286400
H	-3.07635100	-3.10426600	5.92588400
C	-3.63025300	-1.27623200	0.80288000
H	-7.02174200	0.30462300	1.83392000
H	0.01225200	-3.73018700	5.77330400
C	-5.15659900	-0.18915900	4.00441600
H	-5.86699300	-0.86222200	4.50402500
H	-5.47246500	0.83282900	4.24331200
C	-2.74186300	-3.42804400	4.93034400
C	-3.71613800	-2.96416100	3.82901700
H	-4.76230000	-2.94615600	4.14882300
H	-3.64140600	-3.63299900	2.96381600
C	1.90280800	-0.51177200	3.01892000
C	1.99109200	0.87763900	3.28871200
C	3.01499200	-1.20193800	2.47317000
C	0.92020700	1.63318400	3.86816500
C	3.22557400	1.58014800	3.01144700
C	4.25667100	-0.49686100	2.25198200
C	1.04187800	2.97746800	4.11288700
H	0.00029000	1.12350800	4.13086200
C	3.30607900	2.98468300	3.27166500
C	4.32779700	0.87232200	2.52353600
C	2.24639600	3.67063000	3.80050500
H	0.21588600	3.51972200	4.56611100
H	4.23923600	3.49501200	3.04520300
H	5.26196200	1.39848400	2.33850800
H	2.32355800	4.73612800	3.99892600
C	-4.40101000	-1.36223800	-1.63716900
C	-4.16449200	-2.70198700	-2.03934700
C	-4.54058800	-0.34247200	-2.61555600

C	-4.10547400	-3.79500100	-1.11760400
C	-4.00648700	-3.01003200	-3.44238900
C	-4.41789900	-0.67613300	-4.01803500
C	-3.86204000	-5.07484400	-1.54031800
H	-4.26339900	-3.60450000	-0.06307900
C	-3.74432400	-4.35723600	-3.84218900
C	-4.13719900	-1.99313200	-4.39009800
C	-3.66607800	-5.36357000	-2.91991500
H	-3.81641100	-5.88168300	-0.81415200
H	-3.61122400	-4.56182900	-4.90159800
H	-4.03118700	-2.23499100	-5.44558100
H	-3.46297400	-6.38356600	-3.23371500
C	4.05918100	-3.22677500	1.59462000
H	3.97892400	-4.26614500	1.29064300
C	2.96276200	-2.58522500	2.10731100
H	2.02512400	-3.11676300	2.20052700
C	5.29397800	-2.53889500	1.42573100
H	6.14939600	-3.06722700	1.01531800
C	5.38694700	-1.21105000	1.74308600
H	6.31121200	-0.66240800	1.58560800
C	-4.97154800	1.98091400	-3.26736100
H	-5.19069900	3.00828900	-2.98596300
C	-4.87087400	1.63894700	-4.64610500
H	-5.01171800	2.40320200	-5.40539000
C	-4.58944200	0.34764600	-5.00281700
H	-4.49809100	0.06999600	-6.05028100
C	-4.79803100	1.03123000	-2.29103800
H	-4.85762800	1.32139700	-1.24879300
C	-1.68884700	5.68592200	-0.86388500
C	-0.87906200	6.70735800	-0.34716400
C	-2.92901300	6.06033500	-1.41079000
C	-1.28792800	8.04344700	-0.37998300
H	0.08593400	6.48176500	0.09110800
C	-3.33926800	7.39143700	-1.44856600
H	-3.59300100	5.30318300	-1.81905000
C	-2.51776500	8.39424800	-0.93104300
H	-0.63387500	8.80920200	0.02851800
H	-4.30274800	7.64379700	-1.88381500
H	-2.83350800	9.43346900	-0.95844500
C	-2.28406100	3.42059800	0.08551900
H	-3.29864700	3.62487800	-0.27499800
H	-2.12033500	2.34534000	-0.03517100
C	-2.19967000	3.77102100	1.54869000
C	-3.08381300	4.53411700	2.19865000

H	-3.92381400	4.95321300	1.64175500
H	0.41151000	2.63473100	-2.92325300
H	-1.36354200	3.34695700	2.10751500
C	-0.34812000	0.16139800	-3.80156100
H	0.72950400	0.30938000	-3.67415500
H	-0.59494700	-0.85941500	-3.49931700
H	-0.57967100	0.26397900	-4.86833200
C	-3.02648300	4.87900700	3.65885100
H	-2.96214000	5.96550700	3.80689700
H	-3.93171900	4.54551300	4.18450500
H	-2.16160800	4.41852000	4.14856700

INT-14

0 imaginary frequency

H = -5315.384735

G = -5315.587008

E(M06-2X-DCM) = -5316.273549

C	-1.13834200	4.66587800	-0.13786000
C	-1.86855400	4.24253100	1.19298100
H	-1.89003600	3.14802900	1.21461700
H	-1.25367900	4.54566000	2.04435900
C	-3.27755500	4.76967400	1.43132400
C	-1.81938000	3.95454200	-1.33316500
H	-1.35625600	4.26352000	-2.27640100
H	-2.86252300	4.26943600	-1.38518300
N	-1.81706600	2.50024400	-1.21100600
C	-2.77837000	1.68122100	-1.70995800
N	-2.50634900	0.35077500	-1.44625000
C	-3.31160600	-0.79011400	-1.52390600
C	-4.71319800	-0.77688000	-1.62263900
C	-2.65717600	-2.03030200	-1.42209800
C	-5.41948800	-1.97833100	-1.62818000
C	-3.38360000	-3.21843800	-1.42770100
H	-1.57720500	-2.06029600	-1.32060500
C	-4.77333700	-3.21058800	-1.53877600
H	-5.33561100	-4.13600800	-1.55421600
C	-2.66663300	-4.52000700	-1.21376200
C	-6.92521700	-1.93859000	-1.62421700
F	-3.33349800	-5.56924800	-1.73482500
F	-2.50226200	-4.78567600	0.11414000
F	-1.42499200	-4.51833100	-1.75505000
F	-7.41400000	-0.86526100	-2.27319400
F	-7.40898100	-1.88490900	-0.35387800
F	-7.46041100	-3.04186300	-2.19294400

S	-4.11158700	2.24964600	-2.57420400
H	-5.23688000	0.16479900	-1.69758600
C	-4.36367900	4.15026100	0.95267700
H	-1.56163800	0.16653100	-1.10747700
H	-0.98477800	2.06453300	-0.82255100
H	1.74718500	1.57905800	1.35223300
O	0.24383100	-1.47629100	1.13649600
O	2.44597400	-1.27802100	-0.19336400
P	1.19131200	-0.43551200	0.35865900
O	0.35328000	0.34300500	-0.58599400
C	1.65645000	-3.36262200	4.59046000
C	2.06621000	-3.80463700	3.33764900
C	1.50435100	-3.26581600	2.16874500
C	0.17643700	-1.72819000	3.53676300
C	0.68383200	-2.36509600	4.67984700
C	2.25582700	-2.39302400	-1.04194200
C	1.96120200	-3.63181800	-0.47846400
C	1.68776300	-4.70568200	-1.34426100
C	1.78982100	-4.56019600	-2.72281400
C	2.15948200	-3.32510500	-3.25294900
C	2.38665500	-2.21050800	-2.43133900
H	0.32598900	-2.04160300	5.65269000
H	2.25677200	-3.20016400	-4.32727700
C	1.92270700	-4.11510100	0.97120500
C	3.31907400	-4.61223900	1.47072300
H	3.65706900	-5.50886900	0.94197200
H	4.05707500	-3.81944600	1.30320000
H	0.39584200	-6.42156500	-1.01503800
H	2.07098100	-6.67110100	-0.51965100
C	0.65222600	-2.17606900	2.29067000
H	2.08184000	-3.78940100	5.49506100
H	1.57693500	-5.39626900	-3.38358200
C	3.12353200	-4.83108300	2.98923300
H	2.78478900	-5.85284600	3.20841500
H	4.04776200	-4.67647200	3.55681900
C	1.26288000	-5.92786600	-0.56490900
C	0.95189900	-5.33914600	0.82449200
H	1.06826600	-6.05910700	1.63942800
H	-0.08141500	-4.97951300	0.84059200
C	2.77637100	-0.90494500	-3.05501700
C	4.13628500	-0.51289000	-3.05164500
C	1.80266700	-0.11054500	-3.70500300
C	5.17304800	-1.31380700	-2.47397400
C	4.52031200	0.73221900	-3.67681700

C	2. 19994900	1. 13387100	-4. 32558500
C	6. 48234200	-0. 90851600	-2. 49348300
H	4. 90970600	-2. 26217100	-2. 01862000
C	5. 89602600	1. 12264300	-3. 66687500
C	3. 54240000	1. 52278500	-4. 28884700
C	6. 85229300	0. 32966500	-3. 09180700
H	7. 24946400	-1. 53880000	-2. 05160000
H	6. 16641400	2. 06538300	-4. 13675200
H	3. 83619300	2. 45794900	-4. 76184700
H	7. 89490000	0. 63541000	-3. 09589100
C	-0. 84978000	-0. 64456700	3. 64777300
C	-2. 16409300	-0. 87831500	3. 16832400
C	-0. 52123500	0. 59319900	4. 25381300
C	-2. 57669000	-2. 12462200	2. 59742600
C	-3. 15405300	0. 17084900	3. 25977900
C	-1. 53011400	1. 62478500	4. 35806200
C	-3. 85021000	-2. 30785700	2. 12556200
H	-1. 86635500	-2. 94153400	2. 54044100
C	-4. 46819400	-0. 05692500	2. 74272900
C	-2. 81064400	1. 39065700	3. 84993300
C	-4. 81069100	-1. 25850900	2. 18373700
H	-4. 12416400	-3. 26293600	1. 68868000
H	-5. 18936800	0. 75463300	2. 80061000
H	-3. 55746900	2. 17957900	3. 90683800
H	-5. 80238100	-1. 41512600	1. 76988900
C	-0. 49698100	0. 31777000	-4. 41397400
H	-1. 54030400	0. 01938000	-4. 45372700
C	0. 42096100	-0. 48003200	-3. 78263000
H	0. 10342000	-1. 41431900	-3. 33299900
C	-0. 10244900	1. 54986700	-5. 01064600
H	-0. 84876600	2. 17086500	-5. 49739800
C	1. 20858500	1. 94163100	-4. 96756800
H	1. 52437400	2. 87570400	-5. 42633900
C	1. 07114200	2. 10635800	5. 33010400
H	2. 07654500	2. 30585400	5. 68909700
C	0. 06866700	3. 11072000	5. 44664100
H	0. 31100200	4. 06262500	5. 91143800
C	-1. 19289500	2. 87252800	4. 97142000
H	-1. 96991700	3. 62925900	5. 05303000
C	0. 78610200	0. 89368900	4. 75789500
H	1. 56445600	0. 14371400	4. 67894600
N	2. 02980000	0. 59942600	1. 40981800
S	3. 48904400	0. 42972300	2. 24748700
C	4. 83874500	0. 36851100	0. 91411700

O	3.53482700	-0.86479600	2.90869200
O	3.67783800	1.69350300	2.94647700
F	5.90779600	0.98656000	1.41445600
F	5.14397400	-0.89484600	0.64326600
F	4.43763800	0.99549700	-0.18872000
C	0.36478800	4.33023300	-0.03002900
C	1.09990200	4.70192900	1.11203900
C	1.07817500	3.72170700	-1.07670100
C	2.47323700	4.47866300	1.20652100
H	0.60459000	5.19193800	1.94397000
C	2.45560200	3.49787800	-0.98945700
H	0.57262900	3.41352400	-1.98501000
C	3.16197400	3.87680200	0.15091800
H	3.00454100	4.77254500	2.10719000
H	2.96784300	3.01684900	-1.81764100
H	4.23057600	3.69847500	0.22355000
C	-1.31339600	6.21344500	-0.35472100
H	-2.39127200	6.40496900	-0.38416100
H	-0.92494700	6.71551700	0.54104400
C	-0.67822400	6.84760300	-1.58335200
C	-1.38720200	7.03620700	-2.70332200
H	-2.42612700	6.72649100	-2.78712300
H	-4.30457500	3.25415100	0.34233100
H	-5.36312800	4.53322800	1.14690100
H	-0.95251200	7.51063600	-3.57999400
C	-3.40699500	5.99042700	2.31582200
H	-2.98455900	5.79413000	3.31180700
H	-2.86191400	6.85336100	1.91427900
H	-4.45358700	6.28343300	2.44566400
C	0.74755200	7.33528900	-1.47054600
H	1.44732400	6.52020400	-1.25827800
H	1.06995500	7.83204700	-2.39121500
H	0.84490700	8.05494000	-0.64564900

INT-14-1

0 imaginary frequency

H = -5315.381744

G = -5315.583374

E(M06-2X-DCM) = -5316.270080

C	0.20039200	5.15530600	1.22063200
C	-0.77445700	5.04192300	2.44650700
H	-0.24728200	5.41808300	3.33079300
H	-1.58405700	5.75870600	2.26309600
C	-1.40294700	3.69113000	2.77927800

C	-0.54101300	4.80756500	-0.09050700
H	0.11310400	5.00283300	-0.94913400
H	-1.40662200	5.46534500	-0.19758700
N	-1.03710100	3.43897500	-0.16190600
C	-2.12576200	3.04500100	-0.86393200
N	-2.26313500	1.66990700	-0.87226100
C	-3.34097000	0.88758500	-1.30548300
C	-4.68210000	1.28601500	-1.18466900
C	-3.05498900	-0.38957400	-1.80930700
C	-5.69910300	0.42329000	-1.58582600
C	-4.08770200	-1.23967400	-2.20409800
H	-2.02322200	-0.71498600	-1.88870400
C	-5.41916200	-0.84078500	-2.10822800
H	-6.21962600	-1.49571400	-2.43051500
C	-3.76353900	-2.63144800	-2.66510400
C	-7.13555600	0.81430700	-1.35934200
F	-2.57286800	-2.69667200	-3.30661700
F	-4.69977400	-3.13083900	-3.49632700
F	-3.67695700	-3.49913200	-1.61486400
F	-7.30940200	2.14879900	-1.33372100
F	-7.59210100	0.33385200	-0.17108200
F	-7.94958900	0.31074700	-2.31362100
S	-3.16212300	4.12068600	-1.65400900
H	-4.92098300	2.26018200	-0.78311100
C	-0.71353900	2.66736200	3.29964000
H	-1.41572600	1.14121800	-0.65738600
H	-1.20531000	1.73134300	3.54889000
H	-0.49091800	2.72214200	0.30305900
H	1.94543300	0.40570200	1.80200700
O	-0.22250600	-1.92006300	0.52770800
O	1.99835900	-1.64891900	-0.77653800
P	0.94798200	-0.87825200	0.17096700
O	0.34016900	0.38637600	-0.30626400
C	0.58625000	-5.53350500	2.48556100
C	0.90502800	-5.38080500	1.14135800
C	0.52910100	-4.22261900	0.44136800
C	-0.41308900	-3.30084500	2.50529600
C	-0.11080100	-4.51811300	3.13832800
C	1.58020100	-2.13588600	-2.03710500
C	0.94013600	-3.36939300	-2.10106900
C	0.42646700	-3.79293400	-3.33893000
C	0.63179700	-3.04309300	-4.49120800
C	1.35264200	-1.85258400	-4.40980500
C	1.83046000	-1.36063900	-3.18469800

H	-0.40815400	-4.64502500	4.17466300
H	1.53773100	-1.26655500	-5.30504300
C	0.73052400	-4.45955100	-1.05446200
C	1.93277100	-5.45931500	-1.01127200
H	2.02727400	-6.03785100	-1.93534600
H	2.85961000	-4.89113100	-0.87069600
H	-1.29726900	-5.06001900	-3.72093000
H	0.22741200	-5.93637000	-3.57917300
C	-0.02411500	-3.16645000	1.15913400
H	0.86263700	-6.43722100	3.02248800
H	0.23460000	-3.37630400	-5.44630900
C	1.65880700	-6.33014000	0.23497900
H	1.05581400	-7.21354500	-0.01559500
H	2.57957700	-6.69923500	0.70032000
C	-0.34313600	-5.08403300	-3.18497800
C	-0.52699200	-5.17855300	-1.65722700
H	-0.63115100	-6.20461800	-1.29332600
H	-1.42690700	-4.62781900	-1.36729800
C	2.59308800	-0.07220600	-3.16057400
C	4.00161600	-0.09875600	-3.01768700
C	1.91682200	1.15393500	-3.36626500
C	4.74740100	-1.31454800	-2.89387900
C	4.74214500	1.14251900	-3.02847800
C	2.67216300	2.38715300	-3.38791500
C	6.11195600	-1.30509300	-2.76351700
H	4.21564400	-2.25950200	-2.91180500
C	6.16367700	1.10906700	-2.87559300
C	4.05741900	2.34875100	-3.20576700
C	6.83338800	-0.07762200	-2.74482000
H	6.65233100	-2.24396100	-2.67656700
H	6.70288400	2.05340700	-2.87618600
H	4.61915700	3.28058700	-3.21697700
H	7.91440500	-0.08973300	-2.63627600
C	-1.15565100	-2.24364400	3.26129400
C	-2.47174300	-1.88867600	2.86728600
C	-0.57999800	-1.66945700	4.42354300
C	-3.13290700	-2.46262500	1.73468800
C	-3.21294900	-0.92152100	3.64620500
C	-1.34600900	-0.72573400	5.20722900
C	-4.39912500	-2.08110100	1.37549400
H	-2.62218400	-3.21722300	1.14809400
C	-4.52826600	-0.54224900	3.22976800
C	-2.63547800	-0.37726000	4.79669600
C	-5.10628200	-1.09483500	2.11908300

H	-4.86394800	-2.53314200	0.50588500
H	-5.05911700	0.20034700	3.82096600
H	-3.20388600	0.33880000	5.38692000
H	-6.09358700	-0.78219500	1.79208900
C	-0.12120400	2.44376700	-3.76668000
H	-1.19782200	2.48683800	-3.90100100
C	0.49964000	1.24015400	-3.55840400
H	-0.08718100	0.32891300	-3.53943400
C	0.62873200	3.65521500	-3.78662200
H	0.11321000	4.59767400	-3.94653400
C	1.98454200	3.62433600	-3.59888000
H	2.56836600	4.54159600	-3.60816700
C	1.27437700	-1.39064100	5.99391200
H	2.29210800	-1.62569400	6.29199100
C	0.50738100	-0.47769100	6.77100500
H	0.93905400	-0.03416100	7.66404200
C	-0.76484700	-0.15568500	6.38318000
H	-1.36035300	0.54822700	6.95966700
C	0.75046300	-1.96658900	4.86546000
H	1.35630400	-2.65317000	4.28683400
N	1.96507200	-0.56897400	1.49767800
S	3.26760600	-1.40279600	2.17207000
C	4.67990500	-1.26384700	0.92062500
O	2.95916100	-2.82242400	2.24526700
O	3.68160800	-0.60338000	3.31668000
F	4.63939800	-2.28380100	0.07288200
F	4.60383200	-0.10866100	0.26037300
F	5.81775700	-1.30567300	1.61240000
H	0.34909700	2.72786800	3.51231400
C	-2.89725700	3.60169200	2.57438600
H	-3.18881500	3.90391400	1.56147500
H	-3.27129400	2.58911900	2.75508900
H	-3.41712500	4.28329400	3.26343700
C	1.48242300	4.32815800	1.42774200
C	2.02150200	3.50540200	0.42932900
C	2.19511900	4.41746400	2.63857700
C	3.19621500	2.77493100	0.64054200
H	1.53986100	3.41697200	-0.53740700
C	3.36457300	3.69231800	2.85663200
H	1.82963600	5.05774400	3.43630600
C	3.86968900	2.85465300	1.85805500
H	3.58199700	2.15553600	-0.16262100
H	3.88015700	3.77811200	3.80945100
H	4.77591500	2.27995100	2.02661100

C	0.58951700	6.68318700	1.13922900
H	1.14668200	6.92019300	2.05200100
H	-0.34364000	7.25916700	1.18968100
C	1.38626800	7.15079600	-0.07088500
C	2.71423400	7.00405400	-0.14299900
H	3.28751500	6.53409700	0.65079800
H	3.27637600	7.35326300	-1.00614600
C	0.61217900	7.85333400	-1.16315600
H	0.13456100	8.76336100	-0.77382500
H	1.26323300	8.14472100	-1.99348500
H	-0.19572300	7.22987500	-1.56608100

INT-14-2

0 imaginary frequency

H = -5315.381081

G = -5315.582548

E(M06-2X-DCM) = -5316.267415

C	-2.85371600	4.26385800	0.36108500
C	-4.20594300	3.84098500	1.00271400
H	-4.43896800	4.55002900	1.81365500
H	-4.96857800	4.03994600	0.23990000
C	-4.49719000	2.44807800	1.54654800
C	-2.66309600	3.56192400	-1.01515200
H	-1.87029200	4.06510500	-1.58145100
H	-3.57980300	3.66437300	-1.59565400
N	-2.34601500	2.14697400	-0.96044500
C	-3.10752600	1.13981000	-1.45106900
N	-2.49360800	-0.08623400	-1.28091400
C	-2.96192900	-1.38157800	-1.53303800
C	-4.31168600	-1.75988900	-1.44341400
C	-2.00123900	-2.36371800	-1.81716200
C	-4.67319900	-3.08726600	-1.66210400
C	-2.38288800	-3.68803300	-2.02742700
H	-0.95285500	-2.08884600	-1.87286800
C	-3.72285800	-4.06421300	-1.96493600
H	-4.02102700	-5.08970500	-2.14659100
C	-1.32610600	-4.73188700	-2.24565500
C	-6.10746900	-3.50588600	-1.47321800
F	-1.78630900	-5.79974000	-2.92651500
F	-0.84026900	-5.20640600	-1.06194100
F	-0.25739300	-4.24657200	-2.92301200
F	-6.31920400	-3.97942300	-0.21503300
F	-6.45447000	-4.50211000	-2.31872600
F	-6.97115100	-2.49077600	-1.65890200

S	-4.59393100	1.36741800	-2.21984400
H	-5.06212600	-1.01910300	-1.20928400
C	-3.61090900	1.51412500	1.90378000
H	-1.51859300	-0.04626800	-0.98373300
H	-3.94282100	0.55775900	2.29881500
H	-1.44044500	1.89952800	-0.57241800
H	1.37775200	1.60962000	1.83728900
O	0.96953700	-1.55380800	0.72431200
O	2.80620400	-0.24739200	-0.55334200
P	1.42690300	-0.08280400	0.26117500
O	0.27897500	0.58801600	-0.39623800
C	3.43578600	-3.79232400	3.26245300
C	3.74018000	-3.68075600	1.91067000
C	2.85923700	-3.03382100	1.02930800
C	1.38448600	-2.50673200	2.91158000
C	2.24356900	-3.24799400	3.73957700
C	2.83468000	-1.03700300	-1.72833000
C	2.97218100	-2.41709600	-1.60656600
C	2.88012500	-3.20291500	-2.76859300
C	2.74348500	-2.61351800	-4.02023000
C	2.69687400	-1.22361800	-4.11754000
C	2.72704600	-0.40130700	-2.97977100
H	1.97343500	-3.36723000	4.78438700
H	2.61374300	-0.74911900	-5.09072700
C	3.29677500	-3.30508400	-0.40766900
C	4.83942800	-3.45820300	-0.19686600
H	5.31996300	-4.00268900	-1.01556400
H	5.28942600	-2.46028800	-0.14252500
H	2.17341300	-5.24952400	-2.96454200
H	3.90969500	-5.10529400	-2.68455400
C	1.75479300	-2.37695700	1.56003500
H	4.11057100	-4.30543100	3.94272200
H	2.67436700	-3.22585000	-4.91538200
C	4.96951900	-4.16443300	1.17168300
H	4.97071300	-5.25755300	1.06225900
H	5.89512100	-3.89896900	1.69436800
C	2.93266200	-4.67376100	-2.42639900
C	2.69737800	-4.66729300	-0.90313600
H	3.14184600	-5.52480900	-0.38999900
H	1.62158500	-4.68004300	-0.70341300
C	2.67979800	1.08630300	-3.15224800
C	3.87319000	1.83831000	-3.02617500
C	1.47306900	1.71921000	-3.53409500
C	5.14376100	1.23890100	-2.75113200

C	3. 83709500	3. 27023500	-3. 21892000
C	1. 45617500	3. 15050400	-3. 74262300
C	6. 28251000	1. 99481600	-2. 64623000
H	5. 20021500	0. 16249800	-2. 63131700
C	5. 04424500	4. 02427800	-3. 08214300
C	2. 62996900	3. 88624500	-3. 56076900
C	6. 23492500	3. 40912700	-2. 80295200
H	7. 23422300	1. 51151000	-2. 44220400
H	4. 99536000	5. 10194400	-3. 21938800
H	2. 60931700	4. 96360600	-3. 71309400
H	7. 14685200	3. 99248100	-2. 71020800
C	0. 11921800	-1. 93363600	3. 46946800
C	-1. 13119100	-2. 44494600	3. 03674600
C	0. 17235400	-0. 94149900	4. 48072200
C	-1. 25588600	-3. 48347500	2. 05940200
C	-2. 35161400	-1. 92687600	3. 61338600
C	-1. 05753800	-0. 44383600	5. 05652600
C	-2. 48220800	-3. 94496700	1. 65813100
H	-0. 36053400	-3. 91727400	1. 62943400
C	-3. 61157100	-2. 43024400	3. 15961400
C	-2. 28069800	-0. 94512900	4. 60537500
C	-3. 68184900	-3. 40467500	2. 20112500
H	-2. 53672600	-4. 72754900	0. 90874200
H	-4. 51696200	-2. 01583100	3. 59705900
H	-3. 20237600	-0. 56150000	5. 03798300
H	-4. 64212300	-3. 76097500	1. 84068800
C	-0. 89415500	1. 64510900	-4. 14138000
H	-1. 81144200	1. 08294600	-4. 28899200
C	0. 24914600	1. 00419300	-3. 74187700
H	0. 23686300	-0. 06818800	-3. 58345000
C	-0. 90316200	3. 05473100	-4. 34854900
H	-1. 82195200	3. 54116200	-4. 66328500
C	0. 23827600	3. 78321400	-4. 14751300
H	0. 24676500	4. 85925500	-4. 30601000
C	1. 41309800	0. 57793300	5. 94205400
H	2. 36144400	0. 98934500	6. 27515300
C	0. 19924200	1. 05292600	6. 51425400
H	0. 23021500	1. 80990600	7. 29334200
C	-0. 99907600	0. 55549100	6. 07796600
H	-1. 93577600	0. 91046700	6. 50135300
C	1. 39988700	-0. 38287900	4. 96427600
H	2. 33642800	-0. 72688100	4. 54172800
N	1. 99700000	0. 83997100	1. 56525400
S	3. 51990300	0. 98651900	2. 27652900

C	4.58986100	1.86947200	0.98663500
O	4.11631300	-0.32717600	2.45795000
O	3.34907900	1.94747500	3.35867800
F	5.44152000	2.65019100	1.64789600
F	5.26445900	0.97509000	0.27820800
F	3.82706300	2.61803500	0.18793300
H	-2.54051600	1.64003500	1.80353600
C	-5.98076700	2.19676800	1.70535300
H	-6.46196400	2.99085000	2.29442300
H	-6.47519400	2.18188300	0.72526900
H	-6.17757400	1.24094900	2.20038900
C	-1.62936600	4.10209400	1.28140400
C	-0.32722300	4.07863200	0.75554600
C	-1.75730900	4.08327000	2.68091100
C	0.79558500	4.02574500	1.58776400
H	-0.16730600	4.10976700	-0.31816200
C	-0.64236600	4.01654400	3.51541500
H	-2.74361800	4.08904000	3.13117100
C	0.64521400	3.98714200	2.97580200
H	1.78784300	4.02326100	1.14360600
H	-0.78053900	3.97679600	4.59228000
H	1.51574700	3.92945800	3.62162500
C	-2.92024600	5.82070500	0.07055900
H	-1.97250800	6.09138300	-0.40934500
H	-2.92161700	6.32584300	1.04449300
C	-4.06980000	6.36183900	-0.76941700
C	-3.99324300	6.42629600	-2.10411700
H	-3.11916400	6.07926600	-2.64930900
H	-4.80514400	6.83046700	-2.70354600
C	-5.26811700	6.91721000	-0.03359800
H	-4.96405300	7.73854700	0.63039200
H	-6.01967700	7.30500900	-0.72817100
H	-5.75054000	6.16599500	0.60209000

INT-14-3

0 imaginary frequency

H = -5315.381080

G = -5315.582533

E(M06-2X-DCM) = -5316.267416

C	-2.85814400	4.26163100	0.36147900
C	-4.21022000	3.83814400	1.00300000
H	-4.44321800	4.54659500	1.81446000
H	-4.97292600	4.03755600	0.24038900
C	-4.50124900	2.44473600	1.54578600

C	-2.66713700	3.55970800	-1.01470000
H	-1.87489700	4.06349000	-1.58127300
H	-3.58406200	3.66118900	-1.59503300
N	-2.34882600	2.14506300	-0.95958900
C	-3.10878900	1.13719200	-1.45116400
N	-2.49317400	-0.08808300	-1.28177400
C	-2.96015100	-1.38399300	-1.53339000
C	-4.30957700	-1.76359300	-1.44419200
C	-1.99837800	-2.36528500	-1.81682900
C	-4.66968500	-3.09139800	-1.66257400
C	-2.37866300	-3.69002000	-2.02689900
H	-0.95024200	-2.08940800	-1.87213700
C	-3.71828500	-4.06749900	-1.96479900
H	-4.01538600	-5.09332400	-2.14633100
C	-1.32079300	-4.73288700	-2.24454900
C	-6.10356700	-3.51149900	-1.47405000
F	-1.77971900	-5.80133400	-2.92534100
F	-0.83487400	-5.20669900	-1.06057900
F	-0.25233400	-4.24666900	-2.92166000
F	-6.44928300	-4.50812600	-2.31961600
F	-6.96828500	-2.49733000	-1.65997800
F	-6.31510800	-3.98524700	-0.21591400
S	-4.59530100	1.36333500	-2.22018300
H	-5.06087000	-1.02347900	-1.21068300
C	-3.61478200	1.51122500	1.90371400
H	-1.51813900	-0.04686800	-0.98475100
H	-3.94656900	0.55446100	2.29790900
H	-1.44296300	1.89860500	-0.57161600
H	1.37593000	1.61005900	1.83812400
O	0.97101100	-1.55325600	0.72411600
O	2.80644700	-0.24486900	-0.55330900
P	1.42686600	-0.08173800	0.26101800
O	0.27827500	0.58766200	-0.39666700
C	3.43925400	-3.78925800	3.26250600
C	3.74371300	-3.67731000	1.91077300
C	2.86218100	-3.03130000	1.02931800
C	1.38670200	-2.50573600	2.91144800
C	2.24642800	-3.24616300	3.73951000
C	2.83589900	-1.03439800	-1.72831700
C	2.97483000	-2.41435800	-1.60654500
C	2.88379000	-3.20024100	-2.76858800
C	2.74674900	-2.61096200	-4.02024900
C	2.69865400	-1.22112200	-4.11754800
C	2.72775100	-0.39880100	-2.97974300

H	1. 97630300	-3. 36571200	4. 78428600
H	2. 61517400	-0. 74668500	-5. 09073300
C	3. 30024600	-3. 30200900	-0. 40761100
C	4. 84303100	-3. 45337000	-0. 19657600
H	5. 32432300	-3. 99724600	-1. 01523400
H	5. 29186800	-2. 45493800	-0. 14207800
H	2. 17918600	-5. 24754600	-2. 96462200
H	3. 91531900	-5. 10157000	-2. 68459200
C	1. 75699600	-2. 37557300	1. 55992500
H	4. 11447500	-4. 30170300	3. 94284000
H	2. 67846400	-3. 22336300	-4. 91541600
C	4. 97370900	-4. 15955800	1. 17194200
H	4. 97614600	-5. 25266600	1. 06242600
H	5. 89892500	-3. 89309100	1. 69479400
C	2. 93784400	-4. 67104000	-2. 42643900
C	2. 70247700	-4. 66488400	-0. 90318700
H	3. 14794300	-5. 52189900	-0. 39007800
H	1. 62670200	-4. 67893400	-0. 70348500
C	2. 67877300	1. 08876900	-3. 15212400
C	3. 87127400	1. 84216300	-3. 02600500
C	1. 47127700	1. 72030000	-3. 53382000
C	5. 14256200	1. 24419600	-2. 75114300
C	3. 83347800	3. 27407800	-3. 21848000
C	1. 45266200	3. 15162100	-3. 74202100
C	6. 28042700	2. 00142600	-2. 64616900
H	5. 20027400	0. 16783700	-2. 63152600
C	5. 03975200	4. 02951200	-3. 08164600
C	2. 62559100	3. 88872500	-3. 56008600
C	6. 23116900	3. 41570900	-2. 80263800
H	7. 23271900	1. 51920700	-2. 44227800
H	4. 98959100	5. 10714200	-3. 21870100
H	2. 60362800	4. 96609700	-3. 71214200
H	7. 14241900	4. 00011200	-2. 70985200
C	0. 12090600	-1. 93371100	3. 46925300
C	-1. 12906500	-2. 44605600	3. 03649100
C	0. 17316700	-0. 94149100	4. 48048600
C	-1. 25283100	-3. 48483300	2. 05929400
C	-2. 34994900	-1. 92890600	3. 61297200
C	-1. 05718000	-0. 44474500	5. 05611500
C	-2. 47874600	-3. 94744800	1. 65808000
H	-0. 35710100	-3. 91790700	1. 62939000
C	-3. 60946100	-2. 43339800	3. 15922100
C	-2. 27990200	-0. 94699600	4. 60485800
C	-3. 67886100	-3. 40807600	2. 20092400

H	-2.53257100	-4.73019900	0.90882800
H	-4.51522500	-2.01969000	3.59655700
H	-3.20192300	-0.56404100	5.03732700
H	-4.63880900	-3.76532900	1.84056200
C	-0.89586500	1.64349800	-4.14107200
H	-1.81246400	1.08026500	-4.28884700
C	0.24822400	1.00385600	-3.74177800
H	0.23724800	-0.06858300	-3.58365600
C	-0.90659900	3.05316400	-4.34781700
H	-1.82601000	3.53856200	-4.66232700
C	0.23397400	3.78296900	-4.14666000
H	0.24115500	4.85906000	-4.30487900
C	1.41254300	0.57889100	5.94199700
H	2.36052900	0.99100100	6.27526000
C	0.19825300	1.05297400	6.51402700
H	0.22854600	1.80996800	7.29312700
C	-0.99962200	0.55464000	6.07755300
H	-1.93665400	0.90890000	6.50080400
C	1.40020300	-0.38192700	4.96421400
H	2.33706900	-0.72519700	4.54179600
N	1.99613800	0.84159700	1.56498000
S	3.51903700	0.98952500	2.27625500
C	4.58834500	1.87278200	0.98611400
O	4.11658400	-0.32356400	2.45828200
O	3.34736200	1.95082400	3.35797200
F	5.43972200	2.65387400	1.64735500
F	5.26337000	0.97866500	0.27769000
F	3.82518500	2.62093000	0.18749400
H	-2.54434500	1.63778200	1.80474800
C	-5.98483900	2.19243500	1.70284900
H	-6.47828600	2.17820400	0.72227000
H	-6.18159800	1.23603800	2.19678500
H	-6.46703900	2.98569100	2.29221900
C	-1.63371800	4.10041200	1.28179500
C	-0.33156300	4.07846300	0.75584600
C	-1.76158900	4.08060100	2.68127600
C	0.79132100	4.02611700	1.58794900
H	-0.17177800	4.11041900	-0.31785900
C	-0.64652800	4.01442800	3.51568100
H	-2.74787400	4.08511000	3.13159600
C	0.64104300	3.98656900	2.97598400
H	1.78357100	4.02465500	1.14377000
H	-0.78458100	3.97388600	4.59252900
H	1.51164900	3.92943000	3.62174700

C	-2.92542800	5.81842800	0.07100300
H	-1.97797300	6.08956000	-0.40919400
H	-2.92674100	6.32357400	1.04493700
C	-4.07552000	6.35896800	-0.76860700
C	-3.99954900	6.42302600	-2.10336700
H	-3.12555000	6.07615600	-2.64878500
H	-4.81184600	6.82665600	-2.70262000
C	-5.27365200	6.91425800	-0.03245000
H	-6.02607100	7.30066400	-0.72686400
H	-5.75494200	6.16348800	0.60460600
H	-4.96961800	7.73665600	0.63025200

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0 imaginary frequency

H = -5315.380543

G = -5315.582583

E(M06-2X-DCM) = -5316.268253

C	-2.15628700	4.67024200	0.91817500
C	-3.23530700	4.23267100	1.96398300
H	-3.01583800	4.74876500	2.90911100
H	-4.18994900	4.64222900	1.62819300
C	-3.45973200	2.75923400	2.26406600
C	-2.44770900	4.02879900	-0.46190500
H	-1.83714000	4.50996600	-1.23656500
H	-3.48599500	4.21706500	-0.73458400
N	-2.25995100	2.58674700	-0.51594900
C	-3.11621300	1.70833100	-1.09425900
N	-2.63722600	0.41329100	-1.03867700
C	-3.26051300	-0.78628400	-1.40769700
C	-4.63837600	-1.01917300	-1.26492000
C	-2.44158700	-1.82573900	-1.87098600
C	-5.16995700	-2.25852800	-1.61248500
C	-2.99212300	-3.06235100	-2.20794000
H	-1.37314800	-1.66388900	-1.96940800
C	-4.36186400	-3.28942000	-2.09608900
H	-4.79107900	-4.24372300	-2.37678500
C	-2.08611600	-4.18460000	-2.62373700
C	-6.63104600	-2.53497400	-1.37456800
F	-1.60604900	-4.86610200	-1.54280200
F	-1.00014200	-3.74356200	-3.30320300
F	-2.70942300	-5.09171800	-3.40131100
F	-7.37349500	-1.41291400	-1.35749400
F	-6.82535700	-3.15579600	-0.17923100
F	-7.14536600	-3.35561400	-2.31784600

S	-4.56891600	2.15520100	-1.82856500
H	-5.27928300	-0.23520300	-0.88884700
C	-4.66510800	2.21394800	2.06033400
H	-1.65515600	0.31523400	-0.77893500
H	-4.86789600	1.17517700	2.31043000
H	-1.36713900	2.22384800	-0.19690200
H	1.66435200	1.31528900	1.83659100
O	0.73166100	-1.73632700	0.57387600
O	2.63327700	-0.53702300	-0.71133200
P	1.33881300	-0.29210900	0.21569800
O	0.24753900	0.57836600	-0.28528600
C	3.02059000	-4.57441300	2.63530400
C	3.26279500	-4.32598000	1.28943000
C	2.42443200	-3.47115300	0.55521400
C	1.13183700	-3.02102700	2.58548300
C	1.93224600	-3.96151200	3.25475000
C	2.49228200	-1.18085700	-1.96295700
C	2.46076000	-2.57115500	-2.00205000
C	2.20636100	-3.20003100	-3.23309300
C	2.07618100	-2.45642800	-4.40053200
C	2.20118900	-1.06899400	-4.34261500
C	2.39890800	-0.39503800	-3.12678400
H	1.70272400	-4.18477900	4.29211100
H	2.12648700	-0.47799000	-5.25050800
C	2.74001500	-3.62180200	-0.93164600
C	4.26097700	-3.97822400	-0.85074700
H	4.62284000	-4.47061400	-1.75861400
H	4.83353800	-3.05338100	-0.71480200
H	1.23860900	-5.11218200	-3.59788400
H	2.99218800	-5.20774300	-3.42722400
C	1.44680600	-2.75598200	1.23963600
H	3.66076300	-5.24759100	3.19955800
H	1.88094500	-2.94735600	-5.35019200
C	4.37861500	-4.85659700	0.41493600
H	4.23780400	-5.92068800	0.18122500
H	5.35779000	-4.76728900	0.89843900
C	2.09338000	-4.69629600	-3.05570300
C	1.94800600	-4.83802600	-1.52754600
H	2.30992600	-5.79555300	-1.14257500
H	0.89232900	-4.74652500	-1.25507600
C	2.53752700	1.09612800	-3.12791100
C	3.82052700	1.67441500	-2.96874400
C	1.40972900	1.91417400	-3.37632200
C	5.01086000	0.89426100	-2.81366300

C	3.96262100	3.11248900	-2.99704400
C	1.57067400	3.35089000	-3.42428300
C	6.23887700	1.48589000	-2.66853700
H	4.93299500	-0.18731000	-2.81980000
C	5.25955500	3.69011700	-2.82544000
C	2.83481500	3.90930100	-3.21572800
C	6.36834100	2.90383000	-2.66385700
H	7.12599300	0.86789200	-2.55853500
H	5.34523600	4.77409700	-2.83901000
H	2.94799500	4.99117800	-3.24640000
H	7.34930700	3.35490500	-2.54250200
C	-0.02401200	-2.39407700	3.30091600
C	-1.34851500	-2.69890900	2.89430000
C	0.20322900	-1.57715800	4.43717400
C	-1.65112700	-3.55186700	1.78512400
C	-2.46467800	-2.15544900	3.63591000
C	-0.92409900	-1.05828600	5.17950200
C	-2.94443200	-3.81115700	1.41379700
H	-0.83988900	-4.00465500	1.22708400
C	-3.79938900	-2.44235100	3.20809200
C	-2.22180700	-1.36099200	4.75983500
C	-4.03887900	-3.23863700	2.12118300
H	-3.13391600	-4.45601500	0.56229100
H	-4.62275200	-2.00734500	3.76992000
H	-3.06606400	-0.96548900	5.32116300
H	-5.05352000	-3.42865900	1.78442200
C	-0.97013400	2.20631500	-3.85625500
H	-1.95884600	1.78440200	-4.00979700
C	0.09559000	1.38608800	-3.59303600
H	-0.05023600	0.31276200	-3.54983000
C	-0.80326700	3.62042800	-3.91063800
H	-1.66258700	4.25107500	-4.11917100
C	0.43085600	4.17282000	-3.69491100
H	0.57252500	5.25040700	-3.73502000
C	1.69604300	-0.42267400	5.99293500
H	2.70320800	-0.15755900	6.30141400
C	0.58194600	0.07204500	6.72777400
H	0.74654100	0.69862800	7.60012500
C	-0.68951700	-0.23843000	6.32758700
H	-1.55148700	0.13621900	6.87472400
C	1.51394400	-1.21921100	4.89202500
H	2.37692200	-1.58172300	4.34673700
N	2.10245800	0.43767900	1.54737800
S	3.63609800	0.26303200	2.23043800

C	4.84852500	0.98918600	0.97135800
O	3.97796800	-1.14719800	2.32762600
O	3.65696600	1.17905300	3.36299500
F	4.26395100	1.96334500	0.27447900
F	5.87429400	1.48797000	1.65904900
F	5.28259200	0.03479100	0.15820200
H	-5.48545900	2.77297500	1.61875300
C	-2.34826000	1.95214500	2.89026800
H	-1.47501000	1.87225100	2.23284500
H	-1.98902900	2.41246100	3.82019000
H	-2.68355500	0.93778900	3.12170600
C	-0.71120400	4.41802600	1.40018900
C	0.31533800	4.07584900	0.50442000
C	-0.34184100	4.63284100	2.74031600
C	1.63730000	3.91729800	0.93066000
H	0.10498000	3.93279400	-0.55023900
C	0.97320400	4.47110500	3.17365700
H	-1.08969100	4.92564900	3.46953300
C	1.97477300	4.10395500	2.27188300
H	2.39938400	3.65721200	0.20233100
H	1.21625600	4.63337900	4.22034300
H	2.99866700	3.97296700	2.60964500
C	-2.24040800	6.24105400	0.72466400
H	-1.28417800	6.56027800	0.29796700
H	-2.28868800	6.68444500	1.72973700
C	-3.34261800	6.83470500	-0.13923300
C	-3.03273600	7.40900800	-1.30849000
H	-2.01268700	7.43232800	-1.68455800
H	-3.78867600	7.87878800	-1.93308200
C	-4.77020200	6.83826900	0.36043000
H	-5.23619600	5.84808300	0.28453800
H	-4.82508400	7.13800200	1.41486100
H	-5.38607200	7.52959500	-0.22322300

INT-14 欵?0 imaginary frequency

H = -5315.368837

G = -5315.572998

E(M06-2X-DCM) = -5316.267404

O	-0.57388500	-2.34566500	-1.27093700
O	-2.63627100	-1.11333700	-0.28766300
P	-1.00187900	-1.10875100	-0.28046800
O	-0.56299400	0.21990900	-0.82444600
C	-1.64309200	-1.92126600	-5.29821400
C	-2.55363100	-2.41095500	-4.36746900

C	-2.16302100	-2.63280800	-3.03871200
C	0.07040400	-1.79158500	-3.55075700
C	-0.33669000	-1.65360800	-4.89015700
C	-3.34108600	-2.25381500	0.11193300
C	-3.50547400	-3.30534200	-0.79115300
C	-4.07519200	-4.50813300	-0.34348800
C	-4.57117300	-4.62291700	0.95000600
C	-4.50821100	-3.51767800	1.79663200
C	-3.89061700	-2.31693600	1.40791900
H	0.39340200	-1.30707600	-5.61557700
H	-4.92908300	-3.57659500	2.79598800
C	-3.25795500	-3.38838600	-2.29587200
C	-4.51398400	-2.92083400	-3.10665700
H	-4.83502500	-1.94432300	-2.72589600
H	-5.35704400	-3.61140800	-3.00620100
H	-5.03799700	-5.71580000	-1.86607800
H	-3.69793000	-6.53110000	-1.06692300
C	-0.88787700	-2.25161700	-2.62625200
H	-1.93563500	-1.75884600	-6.33255000
H	-5.01464800	-5.55315600	1.29612300
C	-4.01029600	-2.77396000	-4.55982900
H	-4.56157600	-2.01256700	-5.12348800
H	-4.11540200	-3.71512000	-5.11755300
C	-4.04007300	-5.55655300	-1.43359300
C	-3.07316000	-4.93477200	-2.46231500
H	-2.04041900	-5.19404000	-2.20236200
H	-3.25324500	-5.26868500	-3.48895900
C	-3.91878300	-1.16544100	2.36527600
C	-3.20023600	-1.23497800	3.58287900
C	-4.77931200	-0.06868100	2.10882700
C	-2.30134200	-2.30587700	3.89062900
C	-3.35633200	-0.18677300	4.56637500
C	-4.91079700	0.98118200	3.09373500
C	-1.62458000	-2.34751500	5.08053000
H	-2.12900700	-3.07304300	3.14701000
C	-2.63972000	-0.27499200	5.80107600
C	-4.20313400	0.89012600	4.29488000
C	-1.80093800	-1.32536700	6.05586100
H	-0.92630600	-3.15690900	5.27212000
H	-2.77519800	0.51915400	6.53186500
H	-4.31601000	1.67735700	5.03778600
H	-1.25572100	-1.37777400	6.99445400
C	1.49119900	-1.49046900	-3.19161500
C	2.00898700	-0.18674600	-3.39602100

C	2.34876600	-2.53100000	-2.75241300
C	1.19279900	0.92150100	-3.79671300
C	3.41814300	0.06516900	-3.19270000
C	3.74473400	-2.25002600	-2.50395700
C	1.72970200	2.16224700	-4.02758200
H	0.12655300	0.76754900	-3.91090500
C	3.94304200	1.36987600	-3.46352300
C	4.24426200	-0.96668300	-2.74044200
C	3.12730900	2.39119000	-3.87357800
H	1.08360900	2.97973500	-4.33684500
H	5.01271400	1.52586800	-3.34248000
H	5.29921500	-0.76527300	-2.56738300
H	3.54042500	3.37407300	-4.08513700
C	-6.40224200	1.11049600	0.70641100
H	-6.99468100	1.16020600	-0.20348500
C	-5.57108900	0.04037400	0.92013600
H	-5.51590500	-0.75022400	0.18033100
C	-6.50703100	2.15445800	1.66945100
H	-7.17216400	2.99412700	1.48557000
C	-5.78258500	2.08383200	2.82941500
H	-5.86424700	2.86447400	3.58246800
C	2.75926800	-4.85968300	-2.13345800
H	2.39112000	-5.87281800	-1.99641000
C	4.12573700	-4.56902100	-1.86151400
H	4.78611000	-5.35869600	-1.51373700
C	4.60135500	-3.30007300	-2.04839200
H	5.64570600	-3.06435500	-1.85800100
C	1.90578100	-3.87936200	-2.56659100
H	0.87197300	-4.12614000	-2.77639700
C	-1.66763800	3.81608000	-0.73490600
C	-2.33006900	2.94567000	0.38800600
H	-3.41762600	2.99340500	0.27567200
H	-2.06031500	1.90198900	0.20918000
C	-1.97655900	3.30110100	1.82506800
C	-0.15438700	3.95663400	-0.42512800
H	-0.03973100	4.54137200	0.49270700
H	0.34215200	4.49159700	-1.24227200
N	0.55760000	2.68023800	-0.23914400
C	1.79124500	2.61765700	0.22567300
N	2.40724800	1.44478100	0.42005100
C	3.75678900	1.24424900	0.85141700
C	4.81557400	1.58702200	0.01096600
C	3.99459000	0.62616400	2.08417500
C	6.12756300	1.33214600	0.41707200

C	5. 31048400	0. 37662400	2. 47252700
H	3. 16052100	0. 32908700	2. 71222100
C	6. 38105800	0. 73009600	1. 64693900
H	7. 39924900	0. 53620300	1. 96114500
C	5. 58068800	-0. 33003000	3. 77970400
C	7. 24867200	1. 70762300	-0. 51591500
F	5. 57714200	-1. 66903600	3. 62573700
F	4. 65443600	-0. 02532000	4. 70826400
F	6. 79128100	0. 01062800	4. 27909600
F	7. 12495100	1. 07790100	-1. 71277300
F	8. 45835100	1. 39266600	-0. 01861800
F	7. 24449000	3. 03363600	-0. 77986900
S	2. 57856600	4. 16343600	0. 60507800
H	4. 60923700	2. 02466400	-0. 96009200
H	1. 88373100	0. 55983700	0. 29747900
H	0. 09158500	1. 77962700	-0. 46823200
C	-1. 26768100	2. 45245700	2. 58031800
H	-0. 92067400	1. 49055600	2. 21264500
H	3. 69332100	3. 60872600	1. 11798600
H	-1. 04421400	2. 67264200	3. 62160500
N	-0. 57423800	-1. 56967900	1. 20590000
S	0. 93208700	-1. 67490500	1. 67680600
O	1. 14204000	-1. 13038600	3. 02540500
O	1. 91911500	-1. 25969000	0. 63837000
C	1. 21123900	-3. 51425300	1. 85448500
F	0. 99624500	-4. 13619700	0. 69346600
F	0. 37970900	-4. 01965700	2. 77718800
F	2. 47049600	-3. 73614400	2. 24492700
C	-2. 28636900	5. 22956600	-0. 81611500
C	-1. 51675100	6. 39829500	-0. 94435700
C	-3. 68398500	5. 38577600	-0. 81398600
C	-2. 10959700	7. 65954500	-1. 04678300
H	-0. 43322700	6. 35459700	-0. 96062700
C	-4. 27985900	6. 64156100	-0. 91674300
H	-4. 32607700	4. 51688200	-0. 73425200
C	-3. 49597900	7. 78988000	-1. 03134600
H	-1. 47756700	8. 53927600	-1. 13700500
H	-5. 36396500	6. 71905400	-0. 90806700
H	-3. 95936000	8. 76967900	-1. 10836900
C	-1. 77414200	3. 13030200	-2. 15483600
H	-1. 20660600	3. 77291400	-2. 83916800
H	-1. 24819600	2. 17071800	-2. 10178700
C	-3. 13708400	2. 87480700	-2. 77415400
C	-3. 62504300	3. 69754800	-3. 71045400

H	-3.09465000	4.59401500	-4.02140700
H	-4.57871400	3.50625900	-4.19708100
C	-3.86952800	1.61382700	-2.38072900
H	-4.77822000	1.48708500	-2.97903000
H	-3.23317700	0.73189700	-2.52363300
H	-4.15906500	1.60555500	-1.32425700
C	-2.50843400	4.59327500	2.40184800
H	-2.25424900	4.68112800	3.46309900
H	-2.12053600	5.47791700	1.88360400
H	-3.60146000	4.63779400	2.30674300

INT-14欵?1

0 imaginary frequency

H = -5315.366638

G = -5315.568938

E(M06-2X-DCM) = -5316.265704

O	-0.61785900	-2.26352400	-0.95460100
O	-2.78051500	-0.86539100	-0.61544700
P	-1.18963700	-0.90003400	-0.23732400
O	-0.54601800	0.33837100	-0.78087600
C	-0.86814600	-2.51541000	-5.13258300
C	-1.96016500	-2.83080700	-4.33173300
C	-1.84378700	-2.82407300	-2.93438600
C	0.47766600	-2.10223400	-3.12435800
C	0.34202500	-2.19273200	-4.52288700
C	-3.61491100	-1.90955600	-0.20221700
C	-3.63197900	-3.10163500	-0.92766200
C	-4.33419400	-4.20626200	-0.41914700
C	-5.10115100	-4.09249900	0.73419900
C	-5.17916800	-2.85461400	1.36919600
C	-4.44140200	-1.74351200	0.92724400
H	1.21366000	-1.98451800	-5.13577600
H	-5.81188300	-2.73358600	2.24348400
C	-3.08988500	-3.44020600	-2.31241000
C	-4.14530800	-3.11023700	-3.42186800
H	-4.49386100	-2.08102900	-3.27792500
H	-5.01855500	-3.76842500	-3.37749300
H	-5.00719000	-5.65901800	-1.88223300
H	-3.88943100	-6.32356300	-0.69580700
C	-0.65995000	-2.38526000	-2.34265800
H	-0.94637000	-2.53333700	-6.21680800
H	-5.64698000	-4.94617200	1.12804400
C	-3.36299600	-3.21452700	-4.74876600
H	-3.76334800	-2.55696200	-5.52914200

H	-3.39290400	-4.23606100	-5.15324900
C	-4.11385600	-5.42712800	-1.28522600
C	-2.93500000	-4.99280600	-2.18064300
H	-1.98696700	-5.20837400	-1.67458100
H	-2.91637600	-5.49509700	-3.15289200
C	-4.64495100	-0.44138500	1.63699600
C	-4.22578800	-0.28952500	2.98059600
C	-5.39687000	0.58115500	1.00587300
C	-3.45952900	-1.28460300	3.66801700
C	-4.56882500	0.91351900	3.70521200
C	-5.71913100	1.78566800	1.73843600
C	-3.07670500	-1.11238100	4.97162500
H	-3.14812400	-2.16925700	3.12818600
C	-4.15481200	1.05029800	5.06734500
C	-5.29999900	1.91711400	3.06524200
C	-3.43439400	0.06558700	5.68696800
H	-2.46999900	-1.87150700	5.45617800
H	-4.42483800	1.96066400	5.59747300
H	-5.55343100	2.82111100	3.61490900
H	-3.12060200	0.18283600	6.72082900
C	1.82874000	-1.76635100	-2.57758800
C	2.45281700	-0.55490100	-2.97193900
C	2.54778200	-2.70972400	-1.79963100
C	1.75684200	0.48368500	-3.67316600
C	3.84691300	-0.33218100	-2.66488100
C	3.91767200	-2.43194700	-1.42672800
C	2.40270200	1.61700800	-4.09702600
H	0.69345800	0.37145700	-3.84676100
C	4.49069500	0.85129200	-3.15013900
C	4.53961000	-1.27201100	-1.89719100
C	3.79414200	1.79807500	-3.85282300
H	1.85066400	2.38834900	-4.62818400
H	5.55006000	0.97992100	-2.94570100
H	5.58575600	-1.09309600	-1.65832100
H	4.29575300	2.68959600	-4.22034100
C	-6.64746900	1.46413000	-0.90333300
H	-7.02811300	1.34040000	-1.91404200
C	-5.90268200	0.46614200	-0.32931700
H	-5.69788700	-0.43888800	-0.88955900
C	-6.93803600	2.66025500	-0.18636400
H	-7.52902900	3.44185100	-0.65658000
C	-6.48504700	2.81047300	1.09739000
H	-6.71328200	3.71055700	1.66408400
C	2.70762300	-4.83500800	-0.60298400

H	2.25314400	-5.77042700	-0.28848400
C	4.03714900	-4.53109300	-0.19617600
H	4.58157200	-5.22900100	0.43390900
C	4.62478900	-3.36563500	-0.60581300
H	5.64068000	-3.12200300	-0.30528500
C	1.99342600	-3.96051900	-1.37897900
H	0.98394200	-4.21496300	-1.67671200
C	-1.47586500	3.92347300	-0.25911500
C	-2.16853000	3.12771600	0.90991700
H	-3.24760800	3.20059700	0.75824700
H	-1.92059700	2.06855600	0.78693400
C	-1.87258400	3.55786600	2.34301100
C	0.04879100	3.96931400	-0.03888700
H	0.22186600	4.48967300	0.90812500
H	0.52245100	4.56535400	-0.82575200
N	0.72361500	2.65640200	0.03573100
C	1.96423400	2.52770400	0.47101700
N	2.52195000	1.31799900	0.64834100
C	3.88726300	1.01882700	0.92151700
C	4.92313200	1.59649100	0.18007900
C	4.17641600	0.06687700	1.90801900
C	6.24634700	1.25313400	0.46048200
C	5.50255500	-0.28221100	2.15425100
H	3.36606600	-0.40944300	2.44614700
C	6.54620800	0.31752700	1.44863500
H	7.57592300	0.05609600	1.66307800
C	5.82293900	-1.36949000	3.15054200
C	7.35422500	1.81947100	-0.38815200
F	4.84896500	-1.52274300	4.06447700
F	6.97329000	-1.10549500	3.81056700
F	5.99069200	-2.55926000	2.52940700
F	7.59664300	1.03022100	-1.46692000
F	8.51221300	1.91473500	0.29431500
F	7.05001700	3.04637300	-0.86092700
S	2.81841600	4.03631700	0.86806400
H	4.70164100	2.27640500	-0.63357800
H	1.88826300	0.49888900	0.72643200
H	0.21787900	1.79607600	-0.27985500
C	-2.59454900	4.51318500	2.94461000
H	-3.40926600	5.02644800	2.44017500
H	3.85244100	3.43388900	1.48603200
H	-2.40857700	4.80140600	3.97656500
N	-1.14997900	-1.20397800	1.35059400
S	0.16987000	-1.33624200	2.19955100

O	0.08074500	-0.67043700	3.50339900
O	1.42466700	-1.10100800	1.41872300
C	0.25284700	-3.15757100	2.60880700
F	-0.80522400	-3.50344400	3.35707200
F	1.36864000	-3.41058400	3.30186700
F	0.25256700	-3.89624300	1.49663000
C	-1.87343500	3.32165400	-1.62021600
C	-0.94767600	3.10670000	-2.65151200
C	-3.22345900	3.04826700	-1.89725100
C	-1.35354600	2.65358800	-3.90886000
H	0.11092600	3.28368000	-2.49460200
C	-3.63029300	2.58779400	-3.14785400
H	-3.98295700	3.19662800	-1.13726000
C	-2.69749000	2.39256300	-4.16622700
H	-0.61116900	2.50415500	-4.68842600
H	-4.68292800	2.38056100	-3.31920100
H	-3.01242200	2.03725800	-5.14368000
C	-1.96679200	5.41977000	-0.19393600
H	-3.05924000	5.39323300	-0.29202700
H	-1.75293200	5.78486100	0.81509700
C	-0.80994100	2.80455800	3.10878000
H	-1.02700900	1.72989400	3.13660400
H	0.18513900	2.90625000	2.65823600
H	-0.74083200	3.15931300	4.14176700
C	-1.40293700	6.41169300	-1.19970200
C	-0.37869200	7.21066100	-0.87122900
H	0.08794100	7.17455400	0.11096700
H	0.02131300	7.94347600	-1.56788800
C	-2.08375700	6.53060700	-2.54303800
H	-1.63164400	7.32349600	-3.14743500
H	-2.04062800	5.59596800	-3.11084600
H	-3.14827800	6.76864800	-2.41210200

INT-14欵?2

O imaginary frequency

H = -5315.364040

G = -5315.568388

E(M06-2X-DCM) = -5316.264618

O	-0.80498400	-2.39529300	-0.70975100
O	-2.78627400	-0.78116100	-0.23799100
P	-1.16439200	-0.92028900	-0.08225000
O	-0.53484700	0.19311100	-0.86371300
C	-1.53354400	-2.89044700	-4.80554600
C	-2.55859900	-3.03446800	-3.87672200

C	-2.28852500	-2.95878100	-2.50301900
C	0.06121800	-2.51453100	-2.98149100
C	-0.23475200	-2.67335800	-4.34812300
C	-3.63472100	-1.72520300	0.34718600
C	-3.84969900	-2.94464400	-0.29705200
C	-4.57771500	-3.94896900	0.36115100
C	-5.17044000	-3.70725800	1.59491000
C	-5.04938500	-2.44035000	2.16240900
C	-4.28320800	-1.42711100	1.56231200
H	0.58188300	-2.60481800	-5.06052700
H	-5.54513100	-2.21842500	3.10285100
C	-3.51191300	-3.40407800	-1.71253600
C	-4.64614100	-3.02117500	-2.72183500
H	-4.86806000	-1.95358700	-2.60977100
H	-5.57173000	-3.57704100	-2.54218600
H	-5.56851500	-5.38665900	-0.92395700
H	-4.38282500	-6.11215700	0.15641700
C	-1.00893800	-2.61606800	-2.07097100
H	-1.73184500	-2.96293200	-5.87210700
H	-5.73452800	-4.48447900	2.10435100
C	-4.03256200	-3.28199100	-4.11554000
H	-4.44780300	-2.62585000	-4.88937400
H	-4.21536200	-4.31349100	-4.44796200
C	-4.58894200	-5.22427900	-0.45227800
C	-3.49444100	-4.95685800	-1.50540300
H	-2.51651900	-5.24491200	-1.10284300
H	-3.64454400	-5.50475200	-2.44087000
C	-4.27633900	-0.07645500	2.20835600
C	-3.65541100	0.11067500	3.46620900
C	-5.02396200	0.97467600	1.62019500
C	-2.87594000	-0.90801300	4.10211000
C	-3.79153400	1.37756100	4.14990600
C	-5.13973600	2.24033700	2.30897600
C	-2.29076500	-0.69798400	5.32235900
H	-2.71833100	-1.84456200	3.58348200
C	-3.17296400	1.55116700	5.42801300
C	-4.52509800	2.40554500	3.55310300
C	-2.44702000	0.54344600	6.00201000
H	-1.67907100	-1.47850000	5.76478600
H	-3.29157500	2.50829300	5.93082400
H	-4.62227300	3.35791000	4.06999400
H	-1.97550700	0.68920800	6.97019300
C	1.48853400	-2.31058700	-2.58277200
C	2.20495400	-1.19673100	-3.08886500

C	2. 16479600	-3. 29696000	-1. 81971600
C	1. 57313800	-0. 13049400	-3. 80903500
C	3. 63242900	-1. 10576900	-2. 88105900
C	3. 57987000	-3. 15332500	-1. 56032900
C	2. 30146400	0. 90208300	-4. 34261500
H	0. 49477600	-0. 13935600	-3. 91154700
C	4. 35906700	-0. 02359900	-3. 47444900
C	4. 27841100	-2. 07473700	-2. 10961800
C	3. 71758400	0. 95007100	-4. 19338600
H	1. 79586100	1. 69339000	-4. 89086500
H	5. 43759500	0. 00478000	-3. 33869700
H	5. 34749000	-1. 98539700	-1. 93054500
H	4. 28236400	1. 76068400	-4. 64675300
C	-6. 44304000	1. 86861500	-0. 16229100
H	-6. 96607100	1. 72872700	-1. 10503600
C	-5. 71586000	0. 83642100	0. 37337100
H	-5. 66760200	-0. 11229100	-0. 14879300
C	-6. 53200900	3. 12190100	0. 50933100
H	-7. 11299700	3. 92924100	0. 07121800
C	-5. 89871300	3. 29535900	1. 71119900
H	-5. 96935600	4. 24100300	2. 24390100
C	2. 20038600	-5. 39450400	-0. 56496300
H	1. 67901800	-6. 26865200	-0. 18446300
C	3. 58557400	-5. 22856000	-0. 28389200
H	4. 10766500	-5. 97146200	0. 31290500
C	4. 25329100	-4. 14046100	-0. 77535100
H	5. 31505600	-4. 00614700	-0. 58284400
C	1. 51876000	-4. 46759300	-1. 30887000
H	0. 46696800	-4. 62073500	-1. 51711200
C	-1. 46351100	3. 82213500	-1. 11979000
C	-2. 08282200	3. 27610000	0. 22203400
H	-3. 16595900	3. 40201800	0. 15098500
H	-1. 90656100	2. 19680500	0. 26006100
C	-1. 63220000	3. 91308500	1. 53264100
C	0. 07252100	3. 90301900	-1. 01202900
H	0. 30214700	4. 58368900	-0. 18602100
H	0. 47512800	4. 33832500	-1. 93406700
N	0. 73982400	2. 61636300	-0. 75172200
C	1. 98451500	2. 49142500	-0. 31932800
N	2. 46471600	1. 32143700	0. 10768200
C	3. 78731100	1. 11705800	0. 62559000
C	3. 94377300	0. 83138000	1. 98570900
C	4. 88686100	1. 14806300	-0. 22913200
C	5. 22454200	0. 59253000	2. 48324200

C	6.16224300	0.90811300	0.28609200
H	4.74325000	1.34107600	-1.28591100
C	6.33742000	0.63203600	1.64022900
H	7.32920500	0.45440300	2.03808500
C	7.33132000	0.89602200	-0.66275600
C	5.40688400	0.24059000	3.93969400
F	7.33310700	-0.22378400	-1.43330100
F	8.51343200	0.93498600	-0.01905100
F	7.28938000	1.94423800	-1.51433800
F	4.47600700	0.83013700	4.71423000
F	6.62231900	0.62942800	4.38973900
F	5.31775300	-1.09013100	4.14116100
S	3.10677800	3.86885300	-0.21851600
H	3.07563600	0.78242300	2.63464800
H	1.83383200	0.51013700	0.23194200
H	0.18356000	1.73445600	-0.82637200
C	-2.23643300	5.00547600	2.02066800
H	-3.06700900	5.48485100	1.50903500
H	2.35039600	4.71273000	-0.94242300
H	-1.93937400	5.44188800	2.97143100
N	-0.90108400	-1.05234300	1.50679500
S	0.54972400	-1.14657000	2.12876100
O	0.72075300	-0.28022800	3.30401900
O	1.64666400	-1.11033400	1.11895700
C	0.62007300	-2.88803300	2.80235200
F	-0.32108500	-3.05813400	3.74349200
F	1.81906000	-3.10482200	3.35258800
F	0.41829700	-3.77673500	1.82712400
C	-1.93088100	2.96316700	-2.31099000
C	-1.08239800	2.62113700	-3.37347600
C	-3.27474600	2.56376900	-2.40629500
C	-1.55207800	1.91575900	-4.48371300
H	-0.03244000	2.89114200	-3.35289100
C	-3.74656000	1.85667100	-3.51085800
H	-3.97609400	2.79686200	-1.61294000
C	-2.88780200	1.52890400	-4.56025600
H	-0.86623600	1.67118400	-5.29086000
H	-4.79189600	1.56084700	-3.54530100
H	-3.25340500	0.97811300	-5.42255700
C	-1.97837700	5.29764600	-1.33008600
H	-3.06252800	5.22473400	-1.46566500
H	-1.81578700	5.83709400	-0.39104900
C	-0.55423400	3.21522500	2.33064800
H	-0.39420200	3.70742200	3.29466100

H	-0.82209600	2.16983500	2.52757000
H	0.40958700	3.19243300	1.80859700
C	-1.37948600	6.10866000	-2.47079900
C	-1.78713000	5.96866400	-3.73753500
H	-2.55799200	5.25796900	-4.01926600
H	-1.36252100	6.56815900	-4.53966400
C	-0.34488900	7.14612700	-2.09462600
H	-0.77706700	7.89931400	-1.42153700
H	0.50617100	6.71057700	-1.55238500
H	0.04710300	7.66520300	-2.97485800

INT-14欵?3

0 imaginary frequency

H = -5315.367434

G = -5315.571431

E(M06-2X-DCM) = -5316.263663

O	0.80074900	-2.01024300	1.61154300
O	2.79757700	-0.88059200	0.38882200
P	1.16382100	-0.94612500	0.41278300
O	0.66389200	0.43427000	0.72231200
C	1.84404100	-0.81773100	5.48921900
C	2.78363200	-1.40189900	4.64584400
C	2.40365500	-1.88239400	3.38431000
C	0.12019800	-1.11577400	3.77149400
C	0.52061300	-0.71887100	5.06069200
C	3.55033600	-2.04499900	0.19998600
C	3.77050600	-2.89701000	1.28431700
C	4.39488600	-4.13588500	1.06671400
C	4.88452300	-4.47643400	-0.18856900
C	4.76420500	-3.55785200	-1.22904100
C	4.09713900	-2.33165300	-1.06726100
H	-0.23065200	-0.30587300	5.72729400
H	5.18136200	-3.78770400	-2.20497000
C	3.53709200	-2.70126200	2.78073300
C	4.76717000	-2.02022200	3.47005300
H	5.02945300	-1.11600000	2.90863900
H	5.64840000	-2.66896800	3.48812000
H	5.43350600	-4.97598400	2.77423200
H	4.13147300	-5.99722100	2.17324400
C	1.10659000	-1.66203500	2.92613300
H	2.12672600	-0.45669500	6.47489700
H	5.36842600	-5.43520100	-0.35698500
C	4.26156400	-1.63262300	4.87812200
H	4.76633100	-0.74611600	5.27895300

H	4. 42867000	-2. 44295100	5. 60145800
C	4. 42460400	-4. 95412200	2. 33840400
C	3. 43595600	-4. 19414200	3. 24525800
H	2. 41610400	-4. 55002600	3. 05913200
H	3. 64150800	-4. 31359500	4. 31355900
C	4. 09060100	-1. 38612600	-2. 22963900
C	3. 36815500	-1. 70559100	-3. 40414400
C	4. 94084800	-0. 25231600	-2. 20302300
C	2. 48763200	-2. 83097500	-3. 48753200
C	3. 50555800	-0. 87240900	-4. 57779400
C	5. 05618900	0. 58163100	-3. 37883300
C	1. 80764200	-3. 11855200	-4. 64107100
H	2. 33341100	-3. 43918400	-2. 60595400
C	2. 78515400	-1. 21399200	-5. 76518400
C	4. 34187900	0. 24587700	-4. 53283500
C	1. 96263100	-2. 30676600	-5. 80036100
H	1. 12340500	-3. 96143800	-4. 66399100
H	2. 90501100	-0. 57893000	-6. 64000100
H	4. 44462300	0. 86815000	-5. 41990700
H	1. 41475400	-2. 55257700	-6. 70609000
C	-1. 32035100	-0. 98744900	3. 38940500
C	-1. 94261800	0. 28695500	3. 39677800
C	-2. 09280100	-2. 14866900	3. 13034800
C	-1. 22188300	1. 50522500	3. 62339800
C	-3. 36693000	0. 39151400	3. 16881900
C	-3. 50607800	-2. 02135200	2. 85470300
C	-1. 86027100	2. 71856400	3. 67619700
H	-0. 14745100	1. 45758700	3. 75404700
C	-3. 99638900	1. 67580600	3. 24014700
C	-4. 10663900	-0. 76041900	2. 89010900
C	-3. 26995500	2. 80943600	3. 49268800
H	-1. 28549400	3. 62127600	3. 86787000
H	-5. 07425600	1. 72555400	3. 10094800
H	-5. 17384800	-0. 67326300	2. 69805300
H	-3. 76286600	3. 77590200	3. 55690200
C	6. 56403300	1. 19257800	-1. 07875500
H	7. 16081300	1. 42863100	-0. 20168200
C	5. 74095300	0. 09601900	-1. 06710700
H	5. 69633500	-0. 53106900	-0. 18392800
C	6. 65103500	2. 02576000	-2. 22994000
H	7. 30598000	2. 89288700	-2. 22008800
C	5. 91876400	1. 72239800	-3. 34586700
H	5. 98470700	2. 34137000	-4. 23786500
C	-2. 31902000	-4. 57159200	2. 89949600

H	-1.87258700	-5.56189900	2.92509100
C	-3.70285400	-4.43567300	2.59619000
H	-4.29828900	-5.31991700	2.38609600
C	-4.27672800	-3.19409800	2.58123200
H	-5.33575200	-3.07373100	2.36584100
C	-1.54592400	-3.47111400	3.16058800
H	-0.49728600	-3.60067600	3.39912500
C	1.20475800	4.13095800	0.29031700
C	1.78929700	3.30155700	-0.88527400
H	2.87330400	3.46992900	-0.93119900
H	1.69813400	2.24677300	-0.60543100
C	1.21457700	3.44527800	-2.29047900
C	-0.35043300	4.02292900	0.28471200
H	-0.73505300	4.66918300	-0.50498400
H	-0.75564200	4.36989200	1.24088600
N	-0.87754900	2.66763200	0.04750500
C	-2.07863000	2.43378400	-0.45070400
N	-2.53194200	1.18403700	-0.60913600
C	-3.83786200	0.78496000	-1.03523900
C	-4.95234800	1.08067000	-0.24926100
C	-3.96810400	0.01378500	-2.19474600
C	-6.21272500	0.62790600	-0.64275000
C	-5.23423200	-0.43535500	-2.57061000
H	-3.08843000	-0.25050800	-2.77314300
C	-6.36054000	-0.12763600	-1.80419400
H	-7.33914600	-0.47962200	-2.10694100
C	-5.38009800	-1.31022400	-3.79304800
C	-7.40436800	0.98762600	0.20536600
F	-5.19849700	-2.61127600	-3.49219500
F	-4.48405100	-0.98443500	-4.74418900
F	-6.61466800	-1.19412500	-4.33432800
F	-7.14739900	0.79287000	1.52426800
F	-8.49219700	0.25994300	-0.10727900
F	-7.73347900	2.29174800	0.06732600
S	-3.05273200	3.84288700	-0.91980300
H	-4.82567300	1.63755700	0.67253000
H	-1.91721900	0.37666900	-0.39480100
H	-0.31869700	1.84540200	0.34659400
C	0.63151600	4.54111600	-2.79332900
H	0.51400200	5.46368800	-2.23566600
H	-4.02853000	3.12021100	-1.50196300
H	0.26555000	4.55118900	-3.81738400
N	0.75001200	-1.68468100	-0.96187800
S	-0.74783100	-1.94821800	-1.38905100

O	-0.99713500	-1.64615300	-2.80526000
O	-1.75476900	-1.42709800	-0.41829600
C	-0.92799100	-3.80356800	-1.25390000
F	-0.08163900	-4.41441500	-2.09626300
F	-2.17782900	-4.15221600	-1.57572100
F	-0.66562700	-4.21065300	-0.01035600
C	1.55686400	5.63384900	0.24184300
C	0.91031100	6.54328900	1.09804200
C	2.56021400	6.14419400	-0.59412600
C	1.24054300	7.89862600	1.11091300
H	0.14199500	6.19874900	1.78441800
C	2.89708800	7.49905100	-0.58325500
H	3.08221500	5.48747300	-1.27962100
C	2.23940700	8.38551900	0.26779800
H	0.71713100	8.57141400	1.78541400
H	3.67915500	7.85813300	-1.24708500
H	2.50130800	9.44004400	0.27560100
C	1.72106100	3.54541000	1.66069200
H	1.24434000	4.13388300	2.45356900
H	1.34897900	2.51917300	1.75257000
C	3.22532500	3.53899300	1.89548300
C	3.86254900	4.61289000	2.37659900
H	3.34535600	5.54173700	2.59991600
H	4.93441600	4.59914900	2.56055600
C	3.95473700	2.24349600	1.63512500
H	5.02241500	2.33864800	1.85862300
H	3.54157500	1.43557700	2.25338500
H	3.85533300	1.90568000	0.59842300
C	1.38902500	2.20718000	-3.13860900
H	2.44525600	1.91684000	-3.19794500
H	0.86153000	1.34432700	-2.71069100
H	1.02213100	2.36001000	-4.15824600

INT-14欵?4

O imaginary frequency

H = -5315.366059

G = -5315.569567

E(M06-2X-DCM) = -5316.261914

O	0.81241300	-2.24684200	1.34161200
O	2.81463900	-0.91873200	0.36202900
P	1.18198600	-1.00488500	0.33079900
O	0.65591800	0.30576000	0.83636400
C	1.80796100	-1.69438200	5.37334800
C	2.75644300	-2.14436400	4.46075500

C	2. 39481700	-2. 41169700	3. 13228000
C	0. 11026900	-1. 69860800	3. 60565400
C	0. 49256900	-1. 51423200	4. 94696800
C	3. 58522500	-2. 02621500	-0. 01038200
C	3. 79786600	-3. 05026800	0. 91387500
C	4. 43787100	-4. 22810800	0. 49612800
C	4. 95301200	-4. 34022300	-0. 78993100
C	4. 83841400	-3. 25632600	-1. 65798500
C	4. 15215400	-2. 08359700	-1. 29905000
H	-0. 26624300	-1. 20404700	5. 65926100
H	5. 27349600	-3. 31046000	-2. 65142800
C	3. 53945900	-3. 11742500	2. 41686900
C	4. 75764600	-2. 56386600	3. 23091900
H	5. 02786700	-1. 57823400	2. 83457200
H	5. 63932400	-3. 20749700	3. 15304200
H	5. 45104700	-5. 34962300	2. 05138800
H	4. 16685100	-6. 25443300	1. 25688400
C	1. 10503000	-2. 11280300	2. 69786000
H	2. 07790400	-1. 49908800	6. 40819600
H	5. 45102800	-5. 25075600	-1. 11352100
C	4. 22938900	-2. 41825900	4. 67542700
H	4. 72911000	-1. 61528600	5. 22936900
H	4. 38221600	-3. 34061000	5. 25316500
C	4. 45024800	-5. 25514700	1. 60670800
C	3. 43977800	-4. 66822500	2. 61360300
H	2. 42584700	-4. 99019800	2. 34963800
H	3. 62760500	-4. 97089900	3. 64850900
C	4. 13659500	-0. 95232900	-2. 27995500
C	3. 46221800	-1. 09499000	-3. 51682500
C	4. 92368700	0. 19877600	-2. 02590000
C	2. 62970000	-2. 21972500	-3. 81870900
C	3. 59704200	-0. 07019800	-4. 52734900
C	5. 03042400	1. 22702600	-3. 03697400
C	1. 99778800	-2. 33354700	-5. 02859900
H	2. 47071700	-2. 97086500	-3. 05606700
C	2. 93061700	-0. 23420000	-5. 78208400
C	4. 37483200	1. 05976400	-4. 26039000
C	2. 15673800	-1. 33488700	-6. 03065700
H	1. 34872200	-3. 18371100	-5. 21672700
H	3. 04999500	0. 54335100	-6. 53320600
H	4. 47678600	1. 82692400	-5. 02588500
H	1. 64890800	-1. 44481400	-6. 98511700
C	-1. 32358400	-1. 49726200	3. 23082700
C	-1. 93176900	-0. 23146000	3. 42633300

C	-2.10512700	-2.59663100	2.79257200
C	-1.19610700	0.93203300	3.82668100
C	-3.35456200	-0.07918900	3.21833900
C	-3.51665600	-2.41476500	2.53960700
C	-1.82057900	2.13164400	4.05753900
H	-0.12150500	0.85330500	3.94066000
C	-3.96960600	1.18700800	3.48155600
C	-4.10566000	-1.16891800	2.77047900
C	-3.22981400	2.26313200	3.89531200
H	-1.23601000	2.99156300	4.37540500
H	-5.04718000	1.26857800	3.35544900
H	-5.17223400	-1.04405700	2.59698600
H	-3.71151100	3.21520600	4.10169200
C	6.42596000	1.50629400	-0.60620300
H	6.97957900	1.61730800	0.32230700
C	5.66650100	0.38501700	-0.81555200
H	5.62932000	-0.38587700	-0.05448800
C	6.50418000	2.52827400	-1.59436900
H	7.10868900	3.41219500	-1.40960800
C	5.82751700	2.38572200	-2.77533900
H	5.88906200	3.15072500	-3.54620100
C	-2.35092200	-4.95053600	2.18169500
H	-1.91268500	-5.93600300	2.04956000
C	-3.73352200	-4.75683000	1.90503300
H	-4.33623900	-5.59185800	1.55856100
C	-4.29706900	-3.52365700	2.08632800
H	-5.35489500	-3.36211800	1.89308900
C	-1.56912400	-3.91183600	2.61386400
H	-0.52178500	-4.08614000	2.82825900
C	1.22866200	4.04657700	0.67748000
C	1.67475900	3.41803300	-0.67522800
H	2.73202100	3.66042800	-0.84211100
H	1.68129000	2.33279900	-0.52122400
C	0.90689400	3.67306800	-1.96787200
C	-0.31967300	3.90692700	0.84966400
H	-0.80297700	4.67489100	0.24676900
H	-0.59255600	4.07936500	1.89657100
N	-0.87988200	2.60642900	0.44643900
C	-2.08902300	2.44868000	-0.06198900
N	-2.53897000	1.23415800	-0.40232000
C	-3.84508200	0.89249500	-0.87302300
C	-4.95856900	1.06669400	-0.05000900
C	-3.97560400	0.29303800	-2.13004800
C	-6.21768500	0.66701900	-0.50063100

C	-5.24038500	-0.10639000	-2.56239700
H	-3.09663700	0.12250600	-2.74370900
C	-6.36557300	0.08262400	-1.75704700
H	-7.34329500	-0.22887100	-2.10386600
C	-5.38565200	-0.79966400	-3.89620200
C	-7.41001600	0.89850500	0.39019400
F	-6.62257300	-0.61563700	-4.41237500
F	-5.19543200	-2.12923100	-3.78354400
F	-4.49452800	-0.33694300	-4.79383700
F	-8.48621200	0.19347500	-0.00440400
F	-7.76456900	2.20304800	0.41277800
F	-7.14143800	0.55001800	1.67467700
S	-3.08326700	3.90259600	-0.28757300
H	-4.83205300	1.48786900	0.94097700
H	-1.91238500	0.41057400	-0.33222800
H	-0.32340600	1.74697600	0.62061800
C	0.16597500	4.75089800	-2.25812000
H	0.03174700	5.58686700	-1.58076000
H	-4.04550100	3.27622600	-0.99103900
H	-0.32596900	4.83850400	-3.22403400
N	0.80903100	-1.52663300	-1.15032300
S	-0.67731400	-1.70366600	-1.65476300
O	-0.89301200	-1.15434200	-3.00074400
O	-1.70942000	-1.35872300	-0.63275500
C	-0.85643900	-3.55333100	-1.85041200
F	-2.09305800	-3.83633200	-2.27267700
F	-0.63920400	-4.16884100	-0.68623600
F	0.02155500	-4.01221400	-2.75378600
C	1.52561200	5.55606000	0.82486700
C	1.16457100	6.22961800	2.00478100
C	2.15510100	6.30837300	-0.17829700
C	1.41561700	7.59093600	2.17505800
H	0.68988100	5.68826500	2.81852400
C	2.41399100	7.67047800	-0.01015400
H	2.44406500	5.83397100	-1.10884700
C	2.04451700	8.32076400	1.16629100
H	1.12422500	8.07797200	3.10207200
H	2.90632900	8.22132200	-0.80734700
H	2.24545900	9.38057900	1.29686600
C	1.89642200	3.24029100	1.84062400
H	1.52601200	3.64394700	2.79552600
H	1.51041100	2.21598000	1.79213300
C	3.41113600	3.13241800	1.95488300
C	4.30729600	4.01353100	1.49923800

H	4.03819800	4.91393400	0.96139900
H	5.36989400	3.84907600	1.66011200
C	3.85380600	1.89985000	2.71027200
H	4.93505300	1.90004900	2.88123700
H	3.35465500	1.83180800	3.68756500
H	3.58701800	0.99093300	2.15646000
C	1.07934500	2.56899800	-2.98620400
H	0.66117400	1.61746500	-2.63184000
H	0.59781100	2.81756500	-3.93699500
H	2.14173200	2.37722300	-3.18131500

INT-14欵?5

0 imaginary frequency

H = -5315.357181

G = -5315.562215

E(M06-2X-DCM) = -5316.249179

O	3.09467600	-0.44553600	1.37258200
O	3.68183700	-0.54919000	-1.14802600
P	2.60381800	0.09885300	-0.10583500
O	2.61286800	1.57075200	-0.24814300
C	6.60849200	1.47607200	2.58721700
C	6.66266900	0.35588800	1.76419600
C	5.49434900	-0.35252700	1.44574400
C	4.17722000	1.24401500	2.73762100
C	5.37471900	1.88439700	3.09638800
C	3.99694200	-1.90389700	-1.15342300
C	4.93909500	-2.38594600	-0.24354400
C	5.19964800	-3.76431300	-0.19281900
C	4.60660400	-4.63515800	-1.10018700
C	3.73624200	-4.12108100	-2.05966900
C	3.39710300	-2.75779600	-2.10210700
H	5.32191200	2.73660700	3.76782600
H	3.28374100	-4.78565400	-2.78972900
C	5.85598600	-1.65083800	0.73216300
C	7.20693200	-1.22964700	0.06353900
H	6.98672900	-0.69186300	-0.86567600
H	7.83547500	-2.08987500	-0.18816800
H	7.16033500	-4.29987400	0.56232500
H	5.83686300	-4.96863200	1.51190700
C	4.26146100	0.14353800	1.86381100
H	7.51179200	2.02593700	2.83972300
H	4.81749200	-5.70124000	-1.06808300
C	7.86172800	-0.26779800	1.08141000
H	8.50498100	0.47902500	0.60192000

H	8.49273900	-0.81212800	1.79814400
C	6.14946100	-4.08803500	0.93891000
C	6.12093800	-2.79165600	1.77388200
H	5.28105300	-2.82490200	2.47745800
H	7.03451600	-2.62424200	2.35283300
C	2.44644900	-2.28520800	-3.15702200
C	1.11598800	-2.77522300	-3.17541700
C	2.90085000	-1.42622800	-4.18850400
C	0.58395900	-3.62459600	-2.15175600
C	0.23220800	-2.40303900	-4.25700800
C	1.99637300	-1.04038600	-5.24825400
C	-0.69883600	-4.10242800	-2.21254000
H	1.20631700	-3.86670100	-1.29918000
C	-1.09852600	-2.92686200	-4.28589900
C	0.69260000	-1.54237600	-5.25672400
C	-1.55228100	-3.76195600	-3.30047100
H	-1.08169200	-4.73207800	-1.41443800
H	-1.74140300	-2.64815600	-5.11818500
H	0.02218800	-1.26372500	-6.06788700
H	-2.56256900	-4.16064400	-3.33512800
C	2.88344900	1.71593400	3.32479700
C	2.36640800	2.98912900	2.98538300
C	2.22810600	0.91755000	4.29563700
C	2.96197600	3.82492100	1.98564700
C	1.18412700	3.48201700	3.65605400
C	1.02792400	1.40938400	4.93308900
C	2.45613000	5.06623300	1.70254300
H	3.80544300	3.44339100	1.42441400
C	0.69367000	4.78744400	3.33632900
C	0.54556400	2.67882300	4.60351400
C	1.31455700	5.56342900	2.39500700
H	2.91469300	5.67324400	0.92752200
H	-0.18471100	5.15026600	3.86631700
H	-0.34621600	3.05321900	5.10332500
H	0.93632400	6.55571400	2.16269100
C	4.65332800	-0.10675800	-5.26925000
H	5.67905200	0.25158600	-5.29185900
C	4.24424800	-0.93456000	-4.25704900
H	4.95013900	-1.23107600	-3.49030100
C	3.74999900	0.29004800	-6.29577400
H	4.09112000	0.95054000	-7.08854800
C	2.46140700	-0.16973700	-6.28338500
H	1.76296600	0.11416500	-7.06750800
C	2.05988600	-1.11185200	5.65023200

H	2.45505200	-2.08160100	5.94131000
C	0.86484100	-0.63165600	6.25684400
H	0.35575700	-1.23908900	7.00056300
C	0.37015300	0.59578100	5.90791100
H	-0.53500000	0.98150500	6.37197600
C	2.71700300	-0.36364300	4.70863300
H	3.63017200	-0.74274800	4.26429600
C	-2.14507600	3.90692900	-1.26631200
C	-2.01567600	2.85211000	-2.39623000
H	-1.39907300	3.28509800	-3.19384700
H	-1.39391600	2.03834800	-2.00224000
C	-3.22755100	2.20630500	-3.04907100
C	-3.06882400	3.37573800	-0.11152200
H	-4.10958500	3.57897700	-0.35897800
H	-2.83503200	3.90449200	0.81767500
N	-2.94771500	1.93824300	0.16402400
C	-3.94195100	1.06758700	0.22958600
N	-3.65517700	-0.24123900	0.20223000
C	-4.44412700	-1.36592400	0.54565700
C	-5.30206500	-1.38872300	1.65131900
C	-4.26383800	-2.52130500	-0.22452900
C	-6.00753100	-2.55429300	1.94866600
C	-4.96068900	-3.68379400	0.10199600
H	-3.56875000	-2.50846800	-1.05852900
C	-5.84433100	-3.70728900	1.18020600
H	-6.38664900	-4.61170200	1.42599500
C	-4.71705600	-4.92769300	-0.71795000
C	-6.99017400	-2.54766800	3.09367500
F	-3.49489500	-5.44742900	-0.47171600
F	-4.77146600	-4.65782200	-2.04264000
F	-5.62546600	-5.88821200	-0.46008000
F	-7.14763900	-3.77567600	3.62462900
F	-8.20969800	-2.12866000	2.68396000
F	-6.59773900	-1.71554400	4.08096400
S	-5.60312600	1.67766800	0.34911000
H	-5.40038000	-0.52139700	2.29310800
H	-2.70263500	-0.48908600	-0.16234200
H	-1.99847200	1.55849000	0.34829300
C	-4.47506700	2.69150100	-3.05043500
H	-4.74666900	3.62783900	-2.57609800
H	-6.18047300	0.52187400	-0.03332600
H	-5.27430300	2.16806600	-3.57039600
N	1.24444100	-0.77389200	-0.36745700
S	-0.16276400	-0.55501400	0.22007300

O	-1.23002600	-0.98355800	-0.74004500
O	-0.48098500	0.74593900	0.87913000
C	-0.33955300	-1.80448900	1.60269400
F	0.50018700	-1.52832600	2.59539000
F	-0.10148000	-3.03921800	1.14988500
F	-1.60288500	-1.76084600	2.07255100
C	-2.73298800	5.25754100	-1.72180400
C	-3.13014200	6.21179100	-0.76813300
C	-2.84483100	5.61474900	-3.07274600
C	-3.62768000	7.45925000	-1.14536500
H	-3.03909300	5.99654300	0.29289200
C	-3.33951100	6.86275100	-3.45571800
H	-2.55673800	4.91315000	-3.84651200
C	-3.73568900	7.79227600	-2.49555400
H	-3.92522800	8.17147600	-0.38007600
H	-3.41288400	7.10470200	-4.51272800
H	-4.12071000	8.76347400	-2.79411700
C	-0.70962600	4.15920000	-0.65923900
H	-0.83652500	4.82802600	0.19915400
H	-0.32664800	3.21149800	-0.25851500
C	0.33767200	4.76023900	-1.59031600
C	0.45996300	6.08797500	-1.71275700
H	-0.18296000	6.78157200	-1.17755100
H	1.21359400	6.52875800	-2.36121600
C	1.28094400	3.81804500	-2.29951000
H	0.75556400	3.11426900	-2.95746200
H	1.99880000	4.37202300	-2.91347300
H	1.83511400	3.20425900	-1.57945700
C	-2.88899900	0.92396000	-3.77729500
H	-3.76648800	0.49521000	-4.27153400
H	-2.12169800	1.10210200	-4.54322300
H	-2.46506800	0.17371100	-3.09689900

INT-14欵?6

O imaginary frequency

H = -5315.373266

G = -5315.577182

E(M06-2X-DCM) = -5316.267248

O	-0.40476100	-2.76218500	-0.57331900
O	-2.58683800	-1.38258900	-0.29132500
P	-0.96277000	-1.28296500	-0.13693200
O	-0.48991700	-0.20382400	-1.06773000
C	-1.04972000	-3.88841100	-4.55674600
C	-2.04444900	-4.05583200	-3.59918700

C	-1.79195400	-3.75970500	-2.25190400
C	0.46654800	-3.03848500	-2.82877800
C	0.20105400	-3.41972100	-4.15668000
C	-3.30483200	-2.34407400	0.42657700
C	-3.35055800	-3.65694000	-0.04546500
C	-3.93987400	-4.65065400	0.75278800
C	-4.56770600	-4.32415800	1.94914800
C	-4.61860500	-2.98763000	2.34015100
C	-3.98893600	-1.97216100	1.60082100
H	0.99792000	-3.32059700	-4.88776500
H	-5.14246300	-2.70925400	3.24977400
C	-2.94452400	-4.25777900	-1.38908400
C	-4.11709200	-4.18037800	-2.42450200
H	-4.49086500	-3.15043200	-2.45553300
H	-4.95479500	-4.83198500	-2.15709500
H	-4.71403600	-6.37430400	-0.31080000
H	-3.44892700	-6.77385200	0.84640600
C	-0.57571700	-3.18319900	-1.89245200
H	-1.23416600	-4.12871500	-5.60084600
H	-5.02589600	-5.09309700	2.56605600
C	-3.46700500	-4.54006700	-3.77904500
H	-3.96826100	-4.06157800	-4.62828800
H	-3.49929300	-5.62287100	-3.96457600
C	-3.76994300	-6.01556000	0.12307000
C	-2.71375000	-5.74901600	-0.96893000
H	-1.70871100	-5.84078200	-0.54137400
H	-2.77956700	-6.43669400	-1.81779000
C	-4.15136100	-0.55930700	2.07118800
C	-3.56819600	-0.14555300	3.29308000
C	-5.01633100	0.31325900	1.36409400
C	-2.67160600	-0.97432200	4.04043800
C	-3.86753200	1.16652500	3.82145500
C	-5.30442500	1.62378200	1.90335800
C	-2.12535700	-0.54691200	5.22127200
H	-2.39411000	-1.93931700	3.63716400
C	-3.28344900	1.56982700	5.06298300
C	-4.72661800	2.01220200	3.11552100
C	-2.44009000	0.73804600	5.74745700
H	-1.42379900	-1.18572700	5.74945000
H	-3.52271300	2.55888400	5.44662600
H	-4.95666900	2.99500100	3.52275200
H	-1.99594800	1.05811900	6.68616800
C	1.83685800	-2.54925500	-2.48145200
C	2.34705500	-1.38549300	-3.10936100

C	2.66650800	-3.30816400	-1.61758100
C	1.54957100	-0.54373300	-3.95180300
C	3.72557700	-1.00372200	-2.90150900
C	4.02715500	-2.88288900	-1.37837300
C	2.07892500	0.55642900	-4.57586700
H	0.50246500	-0.78642900	-4.08556700
C	4.24780400	0.13713100	-3.59220800
C	4.52411900	-1.75336000	-2.03418000
C	3.45226700	0.89651100	-4.40897800
H	1.44544500	1.17633900	-5.20479100
H	5.29812900	0.38273400	-3.45396700
H	5.55422700	-1.44857400	-1.86360300
H	3.86313400	1.75628800	-4.93194200
C	-6.51119500	0.80626000	-0.51048100
H	-6.98877500	0.49664400	-1.43630300
C	-5.66382800	-0.05342400	0.13995500
H	-5.48067600	-1.03853900	-0.27357100
C	-6.78306700	2.09969000	0.02043100
H	-7.46532600	2.76492400	-0.50226800
C	-6.19639800	2.49041000	1.19521600
H	-6.40947000	3.46765200	1.62351500
C	3.05720300	-5.21853500	-0.14372600
H	2.69554200	-6.12679800	0.33069000
C	4.38622700	-4.77750200	0.11100800
H	5.02440200	-5.34726700	0.78091700
C	4.85494700	-3.64464600	-0.49599800
H	5.87214700	-3.30150900	-0.32249900
C	2.23183800	-4.51360700	-0.97980800
H	1.22729200	-4.87378300	-1.16655900
C	-1.97118800	3.46028900	-1.12535800
C	-2.05588500	3.22479900	0.42264700
H	-3.11131100	3.29426100	0.71018900
H	-1.77404000	2.18512000	0.61717700
C	-1.24316400	4.11459500	1.34961200
C	-0.48773200	3.50797800	-1.57100700
H	-0.05796900	4.45107000	-1.23080000
H	-0.42671300	3.47225400	-2.66382100
N	0.35192100	2.42678300	-1.03310000
C	1.58410500	2.58890700	-0.58687600
N	2.26758000	1.56084400	-0.06663200
C	3.61105300	1.57963400	0.42602800
C	4.68111700	1.70714200	-0.45949800
C	3.83469900	1.39123800	1.79440000
C	5.98792500	1.66893300	0.03165300

C	5. 14626700	1. 35209500	2. 26739900
H	2. 99331300	1. 26400300	2. 46780900
C	6. 22637800	1. 49365000	1. 39317000
H	7. 24106200	1. 47259700	1. 77198500
C	5. 40513800	1. 10767900	3. 73481700
C	7. 12938900	1. 76141500	-0. 94680300
F	6. 56296000	1. 68522200	4. 13037700
F	5. 50671500	-0. 20942800	4. 00453500
F	4. 41660500	1. 60400800	4. 50292500
F	6. 92226400	2. 74008900	-1. 85522800
F	7. 27423300	0. 60821600	-1. 64966100
F	8. 30520000	2. 00555300	-0. 33818600
S	2. 30787000	4. 20703800	-0. 70390300
H	4. 49003900	1. 81406400	-1. 52175400
H	1. 78753700	0. 65967600	0. 10235400
H	-0. 01713900	1. 45263400	-1. 04579400
C	-0. 37853700	3. 56888600	2. 21557700
H	-0. 20678500	2. 49683800	2. 27767900
H	3. 38005200	3. 90958000	0. 05401200
H	0. 16078400	4. 18371600	2. 93334900
N	-0. 69122100	-1. 16515800	1. 45143200
S	0. 75409400	-0. 99887000	2. 06925000
O	0. 80070200	0. 01226200	3. 13674400
O	1. 84343300	-0. 92871900	1. 05333300
C	1. 05321400	-2. 62548400	2. 93972300
F	0. 98737300	-3. 63885900	2. 07423900
F	0. 13292000	-2. 81309600	3. 89734400
F	2. 26386200	-2. 60932200	3. 50642700
C	-2. 66771300	4. 77430100	-1. 54079000
C	-2. 06977200	5. 74444300	-2. 36073500
C	-3. 99098500	5. 01226200	-1. 12705400
C	-2. 75337800	6. 90437000	-2. 73798000
H	-1. 05973700	5. 61290000	-2. 73325300
C	-4. 67501400	6. 16755700	-1. 49941300
H	-4. 50806900	4. 27951400	-0. 51514400
C	-4. 05889900	7. 12569100	-2. 30678300
H	-2. 25645000	7. 63240500	-3. 37400700
H	-5. 69638400	6. 31692600	-1. 15853800
H	-4. 59092300	8. 02726500	-2. 59769600
C	-2. 71524700	2. 24795100	-1. 80441600
H	-2. 25034400	1. 32528900	-1. 44754400
H	-3. 74046300	2. 24086100	-1. 41579800
C	-2. 75230000	2. 21016000	-3. 32416900
C	-1. 86344000	1. 47164800	-4. 00247600

H	-1.10630300	0.88121000	-3.49420100
H	-1.88891800	1.40835400	-5.08850800
C	-3.85591400	2.95356900	-4.04085700
H	-3.82782700	2.75804000	-5.11788400
H	-4.83793800	2.63771200	-3.66315900
H	-3.79777200	4.03618000	-3.88831200
C	-1.50608000	5.60325400	1.35698700
H	-1.24464600	6.08214400	0.40624500
H	-2.57157600	5.81429300	1.51630800
H	-0.93707900	6.09509500	2.15239900

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0 imaginary frequency

H = -5315.368870

G = -5315.572615

E(M06-2X-DCM) = -5316.263912

O	-0.78415900	-2.08625400	-1.55596400
O	-2.79434800	-0.92530400	-0.38651200
P	-1.15926600	-0.98113800	-0.39982600
O	-0.66831300	0.39100100	-0.75569500
C	-1.82005200	-1.05317200	-5.48132400
C	-2.75773100	-1.61402000	-4.62064700
C	-2.37981600	-2.04204500	-3.33990600
C	-0.10334900	-1.26478800	-3.74439200
C	-0.50042500	-0.92210400	-5.04991400
C	-3.54081700	-2.08670800	-0.15617800
C	-3.74959500	-2.98199400	-1.20714900
C	-4.36766600	-4.21514500	-0.94346200
C	-4.86115600	-4.50891800	0.32211700
C	-4.75186000	-3.54923700	1.32618300
C	-4.09220400	-2.32606500	1.11871700
H	0.24990800	-0.52537700	-5.72739100
H	-5.17258100	-3.74283900	2.30843200
C	-3.51088600	-2.84341300	-2.70903100
C	-4.74166000	-2.19513200	-3.42797600
H	-5.00744000	-1.26977400	-2.90409500
H	-5.62063700	-2.84721300	-3.42218500
H	-5.39500100	-5.12703600	-2.62045000
H	-4.08948400	-6.11671300	-1.97569900
C	-1.08784800	-1.79080200	-2.88439500
H	-2.10154500	-0.73271500	-6.48129000
H	-5.34000400	-5.46335600	0.52593000
C	-4.23337600	-1.86187200	-4.84881500
H	-4.74068900	-0.99404300	-5.28565600

H	-4.39450000	-2.70101900	-5.53998600
C	-4.38781100	-5.08251600	-2.18237400
C	-3.40027000	-4.35264200	-3.11478100
H	-2.37909900	-4.69537300	-2.91189100
H	-3.60151900	-4.51464400	-4.17828200
C	-4.09754200	-1.33270900	2.24025700
C	-3.37665100	-1.59595300	3.42951900
C	-4.95542800	-0.20724600	2.16133800
C	-2.49051300	-2.71178100	3.56507200
C	-3.52203300	-0.71230300	4.56453700
C	-5.07745500	0.67832000	3.29792200
C	-1.81274100	-2.94456200	4.73221600
H	-2.33059300	-3.35754500	2.71162600
C	-2.80355600	-0.99715100	5.76790800
C	-4.36371800	0.39881100	4.46715000
C	-1.97550900	-2.08298200	5.85386400
H	-1.12441300	-3.78212800	4.79453800
H	-2.92932700	-0.32459500	6.61340300
H	-4.47249800	1.05923200	5.32551200
H	-1.42921300	-2.28550400	6.77120100
C	1.33306800	-1.10236900	-3.36028700
C	1.93617400	0.18014600	-3.41055500
C	2.12151700	-2.24207500	-3.05816000
C	1.19650300	1.37900500	-3.67692900
C	3.35875000	0.31336200	-3.18718700
C	3.53258100	-2.08459000	-2.78696700
C	1.81708300	2.59901300	-3.77228600
H	0.12235400	1.31079800	-3.80136400
C	3.96902800	1.60359400	-3.30375100
C	4.11511500	-0.81730100	-2.86860300
C	3.22556300	2.71683600	-3.59447000
H	1.22910400	3.48644700	-3.99336400
H	5.04619200	1.67419100	-3.16792200
H	5.18110300	-0.70820700	-2.68110200
H	3.70403300	3.68772700	-3.69241100
C	-6.59093500	1.17057200	0.97354700
H	-7.19241100	1.35981500	0.08832700
C	-5.75832900	0.08216900	1.01106900
H	-5.70938500	-0.58477800	0.15775800
C	-6.68369900	2.05542900	2.08502600
H	-7.34567700	2.91586200	2.03577300
C	-5.94833200	1.81001000	3.21291100
H	-6.01913900	2.46860700	4.07571900
C	2.38110600	-4.65117900	-2.73652000

H	1. 94845500	-5. 64783900	-2. 72453000
C	3. 76285900	-4. 48466900	-2. 43890200
H	4. 37049100	-5. 35205000	-2. 19595700
C	4. 31943300	-3. 23553000	-2. 47037000
H	5. 37658900	-3. 09252900	-2. 25964500
C	1. 59297400	-3. 57216100	-3. 03894700
H	0. 54623900	-3. 72493700	-3. 27203600
C	-1. 24111500	4. 09372300	-0. 36051800
C	-1. 76877800	3. 29836700	0. 86389100
H	-2. 85283100	3. 45169400	0. 94242800
H	-1. 68138700	2. 23643300	0. 60971000
C	-1. 14198200	3. 48115300	2. 24084700
C	0. 31429700	3. 99248600	-0. 42614100
H	0. 73289800	4. 67840600	0. 31065300
H	0. 66997400	4. 29605000	-1. 41636100
N	0. 86308500	2. 65398900	-0. 14967100
C	2. 06625700	2. 44839400	0. 35577500
N	2. 52881800	1. 20828200	0. 55777400
C	3. 83805000	0. 83297800	0. 99448700
C	4. 95023900	1. 11280800	0. 19937200
C	3. 97442800	0. 09904300	2. 17722800
C	6. 21397800	0. 68204600	0. 60617300
C	5. 24402300	-0. 32885500	2. 56622500
H	3. 09684600	-0. 15296100	2. 76428600
C	6. 36776500	-0. 03643600	1. 79025600
H	7. 34904500	-0. 37170100	2. 10318400
C	5. 39655700	-1. 16443600	3. 81501100
C	7. 40343900	1. 02573200	-0. 25159600
F	5. 22229200	-2. 47529800	3. 55499300
F	4. 49959100	-0. 81464300	4. 75676500
F	6. 63097800	-1. 02434300	4. 35089300
F	8. 49213400	0. 30425200	0. 07258100
F	7. 73306400	2. 33220100	-0. 13919000
F	7. 14356000	0. 80577000	-1. 56590000
S	3. 03299400	3. 87892500	0. 77279600
H	4. 81936700	1. 64024200	-0. 73890300
H	1. 91850500	0. 38952300	0. 37609700
H	0. 31291400	1. 81693800	-0. 42260200
C	-0. 51416500	4. 57752800	2. 68580000
H	-0. 39184800	5. 47784900	2. 09381500
H	4. 00477500	3. 18407900	1. 39416400
H	-0. 11331800	4. 61285900	3. 69613900
N	-0. 74770900	-1. 66560500	1. 00321600
S	0. 75008700	-1. 89832500	1. 44742700

O	0.99090100	-1.53550000	2.85090100
O	1.75760100	-1.40944200	0.46042900
C	0.94565800	-3.75612000	1.38937900
F	0.09787000	-4.33887900	2.24987000
F	2.19577900	-4.08126600	1.73400500
F	0.69583100	-4.21535100	0.16147100
C	-1.59240600	5.59619200	-0.34268600
C	-1.02493300	6.46817900	-1.28915900
C	-2.51564800	6.14199900	0.56168900
C	-1.35914400	7.82174400	-1.32896400
H	-0.31993700	6.09240000	-2.02536000
C	-2.85811200	7.49528400	0.52186300
H	-2.96882400	5.51361800	1.31907500
C	-2.28226100	8.34386700	-0.42283500
H	-0.90029600	8.46569600	-2.07481100
H	-3.57728300	7.88381600	1.23820500
H	-2.54800800	9.39701600	-0.45256000
C	-1.81929900	3.44376800	-1.67621700
H	-1.35790900	3.96778800	-2.52509100
H	-1.47427100	2.40599200	-1.71138500
C	-3.32813300	3.44805600	-1.86351400
C	-4.05233400	2.36308900	-1.56398100
H	-3.60490700	1.46003100	-1.15951400
H	-5.12967100	2.34690500	-1.71240500
C	-3.97071200	4.67370500	-2.47214900
H	-3.50282300	4.92138100	-3.43539700
H	-5.03868100	4.50934400	-2.64874800
H	-3.86371300	5.55978500	-1.83766800
C	-1.31618700	2.27800000	3.13860500
H	-0.81433000	1.39061400	2.73032700
H	-0.92080300	2.46125100	4.14249500
H	-2.37543400	2.00874600	3.23370400

INT-14欵?8

O imaginary frequency

H = -5315.365957

G = -5315.571067

E(M06-2X-DCM) = -5316.263482

O	-0.60827400	-2.27252400	-1.34078100
O	-2.67381700	-1.07162700	-0.32522700
P	-1.03936100	-1.07435000	-0.30424200
O	-0.58981400	0.27292700	-0.79090000
C	-1.63939600	-1.68414700	-5.35806500
C	-2.56147100	-2.20224200	-4.45458300

C	-2.18356100	-2.47928900	-3.13256600
C	0.06102000	-1.63959400	-3.59330600
C	-0.33405900	-1.44565100	-4.92953000
C	-3.38650300	-2.22483500	0.02037800
C	-3.54816700	-3.23725100	-0.92655300
C	-4.12748200	-4.45471500	-0.53408200
C	-4.63517800	-4.62076500	0.74921200
C	-4.57464700	-3.55184100	1.64132700
C	-3.94826000	-2.33921500	1.30759000
H	0.40547800	-1.07937400	-5.63537700
H	-5.00526000	-3.64963700	2.63343900
C	-3.28884300	-3.25849000	-2.43099100
C	-4.53553800	-2.75041300	-3.23155600
H	-4.85421900	-1.78859100	-2.81326400
H	-5.38324600	-3.43954400	-3.16652400
H	-5.08369300	-5.59285400	-2.11316900
H	-3.75399400	-6.44760500	-1.33834100
C	-0.90933900	-2.12432500	-2.69425100
H	-1.92180800	-1.47875900	-6.38755400
H	-5.08621500	-5.56223900	1.05249300
C	-4.01890200	-2.54678000	-4.67325500
H	-4.56041400	-1.75872900	-5.20906500
H	-4.12571400	-3.46312600	-5.27056000
C	-4.08850800	-5.45687500	-1.66667000
C	-3.11046600	-4.79757900	-2.66084000
H	-2.08112100	-5.07296600	-2.40397700
H	-3.28393800	-5.08721100	-3.70194700
C	-3.98181200	-1.22689100	2.30908800
C	-3.28721500	-1.35347300	3.53645600
C	-4.82336200	-0.10955900	2.07903800
C	-2.40285400	-2.44415900	3.81613400
C	-3.45206700	-0.34409200	4.55858400
C	-4.95592900	0.90630000	3.09911300
C	-1.75104700	-2.54186100	5.01667500
H	-2.22090200	-3.18025600	3.04386900
C	-2.76247200	-0.49131700	5.80305500
C	-4.27591400	0.75695300	4.31092300
C	-1.93937500	-1.56023000	6.03066700
H	-1.06340400	-3.36482300	5.18803600
H	-2.90461300	0.27359800	6.56309900
H	-4.39177200	1.51745300	5.08064100
H	-1.41453100	-1.65729000	6.97725500
C	1.48401500	-1.37244200	-3.21670900
C	2.02296100	-0.07101400	-3.37685800

C	2. 32454400	-2. 44082800	-2. 81240200
C	1. 22451000	1. 06331700	-3. 73851800
C	3. 43636500	0. 15067500	-3. 16799900
C	3. 72502300	-2. 19101300	-2. 55597800
C	1. 78160600	2. 30203100	-3. 92927800
H	0. 15557800	0. 93106700	-3. 85506700
C	3. 98249400	1. 45465700	-3. 39731300
C	4. 24571600	-0. 90914800	-2. 75145200
C	3. 18314400	2. 50241900	-3. 77139300
H	1. 14871600	3. 13994100	-4. 20971700
H	5. 05493700	1. 58875400	-3. 27439300
H	5. 30425000	-0. 73151100	-2. 57449500
H	3. 61221900	3. 48470900	-3. 95151400
C	-6. 40368100	1. 14426600	0. 69420200
H	-6. 98157800	1. 23522300	-0. 22187100
C	-5. 59415100	0. 05344900	0. 88253800
H	-5. 54046400	-0. 71191200	0. 11671500
C	-6. 50343900	2. 15803500	1. 68978200
H	-7. 14652700	3. 01793700	1. 52219400
C	-5. 79971600	2. 03566000	2. 85739800
H	-5. 87238300	2. 79593300	3. 63131500
C	2. 69773800	-4. 79521900	-2. 27177400
H	2. 31325000	-5. 80625300	-2. 16830500
C	4. 06868200	-4. 53588100	-1. 99104700
H	4. 71627300	-5. 34722800	-1. 67017000
C	4. 56468700	-3. 26927500	-2. 13608800
H	5. 61281200	-3. 05692800	-1. 93902700
C	1. 86013900	-3. 78742900	-2. 67158900
H	0. 82265400	-4. 01077700	-2. 88896600
C	-1. 59401300	3. 89001500	-0. 60332100
C	-2. 31565000	3. 03219200	0. 49194500
H	-3. 39393200	3. 09636800	0. 33014700
H	-2. 05831200	1. 98268400	0. 32226100
C	-2. 01801000	3. 39130300	1. 94898300
C	-0. 08425700	3. 98214600	-0. 26534000
H	0. 02245400	4. 52807700	0. 67764400
H	0. 43378300	4. 54019400	-1. 05304200
N	0. 60157800	2. 68337100	-0. 12472300
C	1. 84418700	2. 58423200	0. 31321500
N	2. 43752000	1. 39463200	0. 47126600
C	3. 78245200	1. 15445100	0. 89696700
C	4. 85058600	1. 50856200	0. 07336400
C	4. 00421600	0. 48835100	2. 10774900
C	6. 15633600	1. 21767000	0. 47598600

C	5. 31367200	0. 20230200	2. 49194100
H	3. 16272200	0. 18421700	2. 72231100
C	6. 39399600	0. 56760900	1. 68420400
H	7. 40735500	0. 34575200	1. 99553700
C	5. 56669500	-0. 55572000	3. 77363700
C	7. 28843000	1. 61081100	-0. 43637500
F	6. 77601500	-0. 24484800	4. 29489100
F	5. 55332800	-1. 88779700	3. 56836800
F	4. 63547800	-0. 27844600	4. 70552200
F	7. 31341300	2. 94727800	-0. 63939400
F	7. 15508700	1. 03915900	-1. 66096300
F	8. 48924400	1. 24757000	0. 04902900
S	2. 66345000	4. 10521900	0. 72229300
H	4. 65649800	1. 98313400	-0. 88274700
H	1. 89325100	0. 52270400	0. 33627000
H	0. 11468300	1. 79973600	-0. 37873500
C	-2. 46486300	4. 51594000	2. 52206100
H	-3. 05987500	5. 24897600	1. 98725200
H	3. 77968900	3. 51825100	1. 19485100
H	-2. 25050400	4. 73423800	3. 56599000
N	-0. 62788900	-1. 59812900	1. 16601200
S	0. 87422700	-1. 73324300	1. 64168500
O	1. 08507300	-1. 24271600	3. 01034300
O	1. 87070100	-1. 28953300	0. 62327800
C	1. 13690300	-3. 58026900	1. 74959800
F	0. 29577400	-4. 11305100	2. 64790600
F	2. 39198500	-3. 82815900	2. 13797500
F	0. 92340700	-4. 15576400	0. 56455200
C	-2. 16683800	5. 32453500	-0. 66160200
C	-1. 36404000	6. 47630000	-0. 68581500
C	-3. 55812500	5. 51824900	-0. 73654600
C	-1. 91892900	7. 75623200	-0. 77062100
H	-0. 28345000	6. 40652500	-0. 63034600
C	-4. 11670700	6. 79221600	-0. 82099700
H	-4. 22454700	4. 66414900	-0. 72918900
C	-3. 29933100	7. 92318400	-0. 83765700
H	-1. 26142300	8. 62175000	-0. 77898200
H	-5. 19713300	6. 89794200	-0. 87440800
H	-3. 73326800	8. 91738700	-0. 90054800
C	-1. 69263300	3. 23502100	-2. 03779900
H	-1. 09068600	3. 87232900	-2. 69717400
H	-1. 19733200	2. 25910800	-1. 99270900
C	-3. 04523800	3. 02743500	-2. 69677200
C	-3. 47364700	3. 86380400	-3. 65006300

H	-2.90319300	4.74121000	-3.94408800
H	-4.41653400	3.70372700	-4.16798600
C	-3.83353000	1.79310100	-2.32674000
H	-4.16882400	1.80222700	-1.28370100
H	-4.71957600	1.69044900	-2.96238900
H	-3.22015800	0.89042900	-2.43539700
C	-1.23660300	2.37228700	2.74531300
H	-1.11175300	2.68481500	3.78662800
H	-1.74238900	1.39955700	2.74264800
H	-0.23938200	2.19457900	2.32461600

TS-EF-5S

l imaginary frequency

H = -5315.361134

G = -5315.560682

E(M06-2X-DCM) = -5316.247128

O	-0.63912400	-2.73118300	-0.51209100
O	-2.76094800	-1.23799300	-0.38120300
P	-1.13219600	-1.20037900	-0.20267700
O	-0.61172900	-0.20648400	-1.19511800
C	-1.25684100	-4.09074300	-4.42457100
C	-2.27036000	-4.16772800	-3.47482000
C	-2.02947500	-3.78789500	-2.14676900
C	0.25889600	-3.16966300	-2.73226700
C	0.00041800	-3.62789500	-4.03688200
C	-3.53436200	-2.11361500	0.38266700
C	-3.62390300	-3.45635800	0.01147100
C	-4.26999300	-4.36038600	0.87038100
C	-4.91234600	-3.91647900	2.02055900
C	-4.91892800	-2.55233100	2.30564800
C	-4.23001700	-1.62451900	1.50644200
H	0.80869300	-3.59406200	-4.76132800
H	-5.45382000	-2.18421800	3.17614800
C	-3.21387400	-4.17791400	-1.27137600
C	-4.36475800	-4.14089900	-2.33386500
H	-4.70273400	-3.10450000	-2.44994400
H	-5.22930200	-4.74212800	-2.03562400
H	-5.08475700	-6.13577600	-0.07014500
H	-3.86024800	-6.48451500	1.14553700
C	-0.79997900	-3.22929600	-1.80607900
H	-1.43267100	-4.39440700	-5.45355600
H	-5.41539300	-4.61627900	2.68302300
C	-3.70382800	-4.62252500	-3.64459000
H	-4.17715800	-4.19738400	-4.53712700

H	-3.76615800	-5.71510300	-3.74638000
C	-4.13723700	-5.77684300	0.35583000
C	-3.04846000	-5.63724300	-0.72828600
H	-2.05682800	-5.73039800	-0.27095200
H	-3.12276400	-6.38816500	-1.52091900
C	-4.34314100	-0.17309000	1.85983900
C	-3.79997200	0.30458000	3.07770800
C	-5.12272100	0.68699500	1.04510200
C	-2.96402000	-0.50041900	3.91614500
C	-4.07573600	1.65842600	3.50504800
C	-5.37229700	2.04602000	1.47356400
C	-2.45881900	-0.01731000	5.09421400
H	-2.69780600	-1.49509600	3.58445100
C	-3.54769800	2.11680900	4.75429500
C	-4.85274800	2.49073700	2.69367600
C	-2.76445200	1.30346400	5.52945500
H	-1.80099900	-0.64133900	5.69143700
H	-3.78615300	3.12901500	5.07428500
H	-5.07202500	3.50405400	3.02663300
H	-2.36560600	1.66438200	6.47375000
C	1.63410700	-2.68695300	-2.39321800
C	2.17148100	-1.56311300	-3.06941500
C	2.43676400	-3.41415300	-1.47850200
C	1.40239900	-0.75370200	-3.96836400
C	3.55159600	-1.19033700	-2.85437100
C	3.80084600	-2.99959600	-1.23929500
C	1.96240600	0.30533500	-4.63561900
H	0.35288000	-0.98342700	-4.10679700
C	4.10315200	-0.08882500	-3.58414700
C	4.32542300	-1.91070900	-1.94091000
C	3.33573200	0.63816000	-4.45430600
H	1.35301900	0.89875200	-5.31247300
H	5.15193700	0.15299300	-3.42912100
H	5.35833700	-1.61323700	-1.77208800
H	3.76695800	1.46978400	-5.00524900
C	-6.47239100	1.11754200	-0.94993200
H	-6.90620900	0.76825200	-1.88273600
C	-5.71761300	0.26444900	-0.18753100
H	-5.56640000	-0.75655400	-0.51763500
C	-6.70136500	2.45876800	-0.53050800
H	-7.30627600	3.11990800	-1.14495100
C	-6.16996500	2.90331600	0.65062800
H	-6.35633600	3.91849700	0.99503300
C	2.77034200	-5.25049100	0.09987900

H	2.38514900	-6.12612100	0.61556000
C	4.10345400	-4.82006100	0.35185800
H	4.72105000	-5.36430500	1.06109300
C	4.60151500	-3.72882700	-0.30592500
H	5.62125400	-3.39337200	-0.13285100
C	1.97050900	-4.57631400	-0.78501500
H	0.96229200	-4.92836000	-0.96858400
C	-1.62386700	3.53882700	-1.09060400
C	-1.64076800	3.24337400	0.44030100
H	-2.62900300	3.50331900	0.85022000
H	-1.58086900	2.16106300	0.60080200
C	-0.65391900	3.89267200	1.36089200
C	-0.18088500	3.32268900	-1.65326300
H	0.39816200	4.24124100	-1.60229000
H	-0.24663500	3.04807800	-2.71073600
N	0.60411400	2.30441400	-0.95654600
C	1.86679300	2.46935100	-0.52081100
N	2.50739100	1.36595300	-0.08660600
C	3.84639500	1.32226000	0.40444700
C	4.91088100	1.53391400	-0.46901800
C	4.08237900	0.97897700	1.73778100
C	6.22044300	1.39637400	-0.00848900
C	5.39775800	0.85848800	2.18852600
H	3.24653700	0.80877100	2.40712000
C	6.47227500	1.06193100	1.32077800
H	7.49035300	0.96269800	1.67703300
C	5.66263900	0.44699000	3.61430300
C	7.34280900	1.53473700	-1.00001000
F	5.72090800	-0.89708200	3.74148700
F	4.69835900	0.88463000	4.44950700
F	6.84272400	0.93552200	4.06074000
F	7.35122400	0.48878800	-1.87257400
F	8.55334500	1.56530000	-0.40936100
F	7.21995800	2.65201200	-1.74708600
S	2.62869200	4.02874700	-0.42095000
H	4.71109000	1.77712900	-1.50599800
H	1.99685000	0.47952500	0.01190600
H	0.23741200	1.33730100	-1.01515500
C	0.07480200	5.05104500	1.03683200
H	-0.32558500	5.69235400	0.25239000
H	1.10559500	4.61112600	0.47066900
H	0.51703100	5.58825900	1.87755600
N	-0.88551100	-0.97003500	1.38184700
S	0.55736900	-0.96029100	2.03328300

O	0.68843100	0.10138600	3.04856200
O	1.67543900	-1.08861100	1.06315900
C	0.62200000	-2.55014700	3.01490900
F	0.45644800	-3.60199600	2.21119200
F	-0.34629000	-2.55976500	3.94508800
F	1.80448400	-2.64585300	3.62844200
C	-0.43097600	3.21312400	2.66458400
H	0.20311400	3.79554700	3.33686200
H	-1.39422500	3.01305900	3.15495700
H	0.01374000	2.21478400	2.52717800
C	-2.63793100	2.50411400	-1.72080200
H	-2.35556800	1.50609700	-1.37322700
H	-3.62322500	2.71886300	-1.29356800
C	-2.74546700	2.47216200	-3.24027100
C	-3.44848700	3.38136200	-3.92637800
H	-3.97035000	4.19997700	-3.44011900
H	-3.53177900	3.33000400	-5.00974200
C	-2.08843700	1.30290700	-3.93737100
H	-1.01972600	1.22173000	-3.70583200
H	-2.53037800	0.35793000	-3.59573300
H	-2.20594600	1.36825600	-5.02414000
C	-2.11732000	4.96754600	-1.40924200
C	-3.26992200	5.47360200	-0.78185300
C	-1.50242400	5.78537100	-2.37086900
C	-3.76476400	6.74342000	-1.07538800
H	-3.81361100	4.86525400	-0.06498400
C	-1.99385700	7.05951800	-2.66727000
H	-0.63483900	5.43674200	-2.91929500
C	-3.12389600	7.54977800	-2.01733400
H	-4.65637600	7.10081100	-0.56668500
H	-1.48873500	7.66303500	-3.41663100
H	-3.50592200	8.54081800	-2.24585500

TS-EF-5S-1

l imaginary frequency

H = -5315.354653

G = -5315.555019

E(M06-2X-DCM) = -5316.242912

O	-0.69168700	-2.45675300	-1.14695900
O	-2.71362600	-1.03132000	-0.34387600
P	-1.07856900	-1.10861700	-0.29975000
O	-0.56578000	0.14096100	-0.95549300
C	-1.61467800	-2.40397900	-5.23130200
C	-2.57910800	-2.73962500	-4.28668900

C	-2.23903200	-2.84089200	-2.93012600
C	0.05227600	-2.17491500	-3.44805900
C	-0.30755700	-2.16353300	-4.80807200
C	-3.48385400	-2.09290400	0.13654200
C	-3.67960900	-3.21645900	-0.66959600
C	-4.32463400	-4.34105700	-0.12943700
C	-4.85962700	-4.30954000	1.15300700
C	-4.75931400	-3.13521000	1.89590300
C	-4.06969200	-2.00878800	1.41615800
H	0.46162400	-1.93621400	-5.54019100
H	-5.20831600	-3.07971200	2.88314600
C	-3.39514700	-3.45693700	-2.15179500
C	-4.59927100	-3.00295900	-3.04449400
H	-4.86851800	-1.97523000	-2.77459400
H	-5.48541400	-3.62934900	-2.90197600
H	-5.31271800	-5.63498900	-1.56072600
H	-4.04200900	-6.44067500	-0.64661500
C	-0.95751500	-2.48617900	-2.51601500
H	-1.86657400	-2.33933300	-6.28694700
H	-5.36085500	-5.17972000	1.56921800
C	-4.04964300	-3.03610000	-4.48837000
H	-4.53889200	-2.30559500	-5.14296600
H	-4.19839000	-4.02160100	-4.95153200
C	-4.31895700	-5.48894300	-1.11426400
C	-3.29248400	-5.01995800	-2.16510600
H	-2.28292100	-5.30689100	-1.84939400
H	-3.46302200	-5.44068400	-3.16086700
C	-4.07208600	-0.77734200	2.27064600
C	-3.40727300	-0.78044700	3.52127600
C	-4.87518400	0.33013200	1.89635000
C	-2.55676900	-1.85325400	3.93989200
C	-3.57173000	0.33748400	4.42435500
C	-5.00840300	1.45429500	2.79703800
C	-1.93514300	-1.83405900	5.16017100
H	-2.37479700	-2.67134200	3.25572000
C	-2.91827700	0.30951800	5.69676200
C	-4.36316100	1.42316100	4.03731000
C	-2.12608500	-0.74597000	6.05827700
H	-1.27003800	-2.64672100	5.43585500
H	-3.06363500	1.15225200	6.36904600
H	-4.49266100	2.25797800	4.72422000
H	-1.62860100	-0.75275800	7.02435900
C	1.47237200	-1.89570300	-3.06847100
C	2.05765900	-0.64688300	-3.39845300

C	2. 26215300	-2. 91023200	-2. 47026400
C	1. 31484600	0. 43624500	-3. 97273200
C	3. 46447600	-0. 42601100	-3. 14854900
C	3. 65536700	-2. 65496400	-2. 18146000
C	1. 91814300	1. 61904900	-4. 31605100
H	0. 25155300	0. 30952500	-4. 13448700
C	4. 06060600	0. 81640800	-3. 53770500
C	4. 22101400	-1. 42711400	-2. 53449300
C	3. 31432300	1. 81223200	-4. 10934200
H	1. 32652700	2. 41762000	-4. 75678700
H	5. 12691800	0. 94611600	-3. 36886400
H	5. 27267500	-1. 24327700	-2. 32530600
H	3. 78066300	2. 74791700	-4. 40643200
C	-6. 40025800	1. 45132300	0. 34643100
H	-6. 95283900	1. 45239200	-0. 58893000
C	-5. 61265600	0. 37683700	0. 66968000
H	-5. 54950300	-0. 46421700	-0. 01080100
C	-6. 50609600	2. 56701700	1. 22541200
H	-7. 13852300	3. 40877300	0. 95528300
C	-5. 82762500	2. 56345200	2. 41531500
H	-5. 91596100	3. 39877100	3. 10679700
C	2. 54130100	-5. 16544600	-1. 56983700
H	2. 12361500	-6. 14180100	-1. 33921200
C	3. 90395300	-4. 89632800	-1. 25928900
H	4. 51165200	-5. 66414400	-0. 78835100
C	4. 44230000	-3. 67611500	-1. 56350300
H	5. 48479500	-3. 45820800	-1. 34437200
C	1. 75301000	-4. 21061900	-2. 15636900
H	0. 72130000	-4. 44199600	-2. 39293200
C	-1. 56866100	4. 07590200	-0. 48460100
C	-1. 54762300	4. 39882400	1. 06896400
H	-1. 24967300	5. 44638500	1. 17188400
H	-2. 58222400	4. 32776700	1. 42959800
C	-0. 69870400	3. 57966700	2. 00265500
C	-0. 11747200	3. 80238200	-0. 96260200
H	0. 51228000	4. 66765000	-0. 75639300
H	-0. 11318200	3. 63773200	-2. 04333200
N	0. 53367800	2. 63664100	-0. 35036900
C	1. 80837900	2. 60203400	0. 07757600
N	2. 39777300	1. 40588700	0. 22378700
C	3. 73309700	1. 20135500	0. 70323800
C	4. 80722700	1. 51742800	-0. 12422700
C	3. 94525000	0. 62036600	1. 95432200
C	6. 10865700	1. 24999800	0. 30148500

C	5.25351100	0.37101700	2.37294800
H	3.10091200	0.35708600	2.58250200
C	6.33928400	0.67958400	1.55188800
H	7.35038100	0.47971400	1.88450400
C	5.48708500	-0.29112300	3.70759900
C	7.24255600	1.53193100	-0.64574800
F	6.72638400	-0.02852900	4.18304300
F	5.37167200	-1.63339900	3.62401900
F	4.59935500	0.12875000	4.63246800
F	7.22670600	0.67021500	-1.70010700
F	8.44837100	1.41340200	-0.05747900
F	7.15965400	2.77353700	-1.17056700
S	2.62590500	4.05713700	0.59176800
H	4.62109800	1.94805500	-1.10135500
H	1.87644100	0.53881900	0.03989000
H	0.11494100	1.71657600	-0.58062900
C	0.37292500	4.20411100	2.63388600
H	0.35791900	5.29266700	2.71029800
H	1.36450400	4.18411600	1.69387600
H	0.85644100	3.68955200	3.46421500
N	-0.71402000	-1.43592800	1.23852800
S	0.78038400	-1.54081600	1.75712000
O	0.97368800	-0.82179400	3.02828500
O	1.80850600	-1.32311600	0.70665200
C	0.95766900	-3.34767400	2.20085300
F	0.74681500	-4.11289900	1.12790600
F	0.07273700	-3.68528700	3.15208000
F	2.19029900	-3.57118800	2.66554400
C	-2.10942100	5.35904000	-1.15383400
C	-3.39408900	5.81819200	-0.81252400
C	-1.37804700	6.11723100	-2.07897300
C	-3.92134000	6.98261300	-1.36442300
H	-4.00075000	5.25490000	-0.10925900
C	-1.90634800	7.28453000	-2.63930600
H	-0.38256900	5.81525100	-2.38441200
C	-3.17801500	7.72521400	-2.28428200
H	-4.91800500	7.30794600	-1.07795400
H	-1.31213300	7.84725100	-3.35441500
H	-3.58751200	8.63343200	-2.71773700
C	-2.54206200	2.87952100	-0.79483900
H	-3.41051700	2.97756700	-0.13629300
H	-2.05818500	1.93666000	-0.52114600
C	-3.05679800	2.73557200	-2.21977100
C	-4.35954000	2.87943600	-2.48520200

H	-4.75424200	2.73168900	-3.48785600
H	-5.07867700	3.14129700	-1.71482000
C	-1.06476300	2.17115900	2.34009200
H	-0.22172700	1.59262500	2.72833000
H	-1.82003800	2.20732100	3.14066500
H	-1.52293000	1.62546000	1.51562700
C	-2.08607100	2.34754100	-3.30987900
H	-1.44293500	3.18920600	-3.60198500
H	-1.43632900	1.52886300	-2.98090000
H	-2.61898300	2.02698300	-4.21077200

TS-EF-5S-2

l imaginary frequency

H = -5315.353530

G = -5315.553736

E(M06-2X-DCM) = -5316.240010

O	-1.08234400	-2.00554800	-1.62250200
O	-2.91257600	-0.68342900	-0.33594300
P	-1.28880200	-0.90107200	-0.42812500
O	-0.69351700	0.43189900	-0.77015100
C	-2.22679400	-0.81162400	-5.46688300
C	-3.16106400	-1.32376600	-4.57201500
C	-2.75563200	-1.79937800	-3.31682500
C	-0.45002600	-1.16856300	-3.81679300
C	-0.88248900	-0.77274000	-5.09526600
C	-3.75223300	-1.77061800	-0.07661500
C	-4.09219300	-2.63607500	-1.11821100
C	-4.80231200	-3.81165000	-0.82405200
C	-5.25958500	-4.06545300	0.46387500
C	-5.01579900	-3.12552400	1.46389000
C	-4.25714200	-1.96792400	1.22497300
H	-0.13989900	-0.40811100	-5.79891700
H	-5.40295900	-3.28762300	2.46556700
C	-3.91368100	-2.51476500	-2.63162900
C	-5.12396600	-1.76956900	-3.29047000
H	-5.29480800	-0.83065800	-2.75092600
H	-6.04895400	-2.35283300	-3.24561500
H	-5.97577900	-4.63292400	-2.45224600
H	-4.72999400	-5.72811200	-1.86251200
C	-1.42773600	-1.65147200	-2.92468900
H	-2.53152000	-0.45544900	-6.44787400
H	-5.81032600	-4.97498400	0.69006800
C	-4.65954800	-1.46509400	-4.73262900
H	-5.12542800	-0.56252800	-5.14478700

H	-4.91106300	-2.28802000	-5.41630600
C	-4.95003900	-4.67261800	-2.05914800
C	-3.94652100	-4.02726400	-3.03681100
H	-2.94947800	-4.45370000	-2.87792200
H	-4.20783600	-4.17164600	-4.08978000
C	-4.09638100	-0.98319700	2.34373800
C	-3.31918400	-1.31144000	3.48065000
C	-4.84187900	0.22232100	2.31563900
C	-2.55038400	-2.51538800	3.56939800
C	-3.28135400	-0.40591900	4.60791400
C	-4.78182800	1.12735300	3.44201000
C	-1.81512100	-2.80962800	4.68660300
H	-2.52582900	-3.18214500	2.71782600
C	-2.50792800	-0.75578100	5.75908400
C	-4.00419900	0.78957100	4.55438300
C	-1.79814900	-1.92477200	5.80170400
H	-1.21757700	-3.71568800	4.71174000
H	-2.49752700	-0.06710500	6.60103600
H	-3.98014700	1.46339400	5.40928600
H	-1.20945900	-2.17765200	6.67940300
C	1.00505200	-1.09490900	-3.47602900
C	1.67309800	0.15579000	-3.49099500
C	1.73592600	-2.28369100	-3.22430600
C	0.99711700	1.40009600	-3.71513000
C	3.10156100	0.20777900	-3.26986700
C	3.15502100	-2.20906300	-2.95984600
C	1.68169500	2.58783900	-3.77497200
H	-0.07962500	1.39204500	-3.83660700
C	3.77832200	1.46757500	-3.34021600
C	3.80058700	-0.97059100	-2.99617100
C	3.09457500	2.62661000	-3.59355300
H	1.14296400	3.51234600	-3.96887700
H	4.85677000	1.47661600	-3.19705300
H	4.87094500	-0.92035000	-2.80710100
H	3.62159600	3.57486000	-3.65598900
C	-6.43286400	1.73983800	1.24319500
H	-7.08792900	1.97603700	0.40876800
C	-5.70560400	0.57781700	1.22980300
H	-5.79200000	-0.09999100	0.38803500
C	-6.34780700	2.63955900	2.34321500
H	-6.92986900	3.55720300	2.33612200
C	-5.54533900	2.33643300	3.40969500
H	-5.48325300	3.00587400	4.26492100
C	1.87119600	-4.71254300	-2.98762000

H	1.38717400	-5.68528300	-3.00581100
C	3.26212700	-4.62858100	-2.69771600
H	3.82528200	-5.53423400	-2.48985900
C	3.88289300	-3.40970400	-2.69071600
H	4.94707300	-3.32891000	-2.48284200
C	1.13823100	-3.58410900	-3.24501900
H	0.08286400	-3.67359900	-3.47329500
C	-0.83422000	4.37754600	-0.01467500
C	-1.16429700	4.29662500	1.54014000
H	-1.04371100	5.29062900	1.97338800
H	-2.22638500	4.04265100	1.62132800
C	-0.40198000	3.32247700	2.39991200
C	0.61744600	3.90457500	-0.33554900
H	1.33997400	4.58872500	0.10449100
H	0.74572300	3.95379300	-1.42364600
N	0.98236400	2.54704900	0.09043400
C	2.18891800	2.21679000	0.58711300
N	2.58305500	0.93759500	0.51883600
C	3.87249900	0.46007500	0.91861500
C	4.98172100	0.80494500	0.15002700
C	3.99953600	-0.41176800	2.00067700
C	6.23379000	0.27835500	0.46635900
C	5.26132400	-0.92077600	2.31396400
H	3.12383000	-0.69953700	2.57313300
C	6.38152000	-0.58244500	1.55224600
H	7.35381400	-0.99073400	1.79899900
C	5.40072800	-1.89877500	3.45367600
C	7.40483700	0.65298800	-0.40060300
F	6.65844900	-1.90329100	3.95320000
F	5.12710000	-3.16120900	3.06134700
F	4.56151500	-1.60442600	4.46715200
F	7.11286200	0.47394600	-1.71723200
F	8.50122900	-0.08124400	-0.12925600
F	7.74109700	1.95351200	-0.25877000
S	3.15484000	3.39249700	1.44250800
H	4.85554100	1.45915200	-0.70524000
H	1.96186900	0.20755500	0.14278900
H	0.43127200	1.77333900	-0.31728100
C	0.67115400	3.76963300	3.16736900
H	0.75396600	4.84067200	3.35835000
H	1.76083100	3.66465500	2.35887700
H	1.01677100	3.13204700	3.98180300
N	-0.88487000	-1.65993100	0.93652100
S	0.60804800	-2.05116700	1.29136700

O	0.94944200	-1.72528500	2.68515900
O	1.60319600	-1.66814300	0.25408200
C	0.59426800	-3.91893700	1.22551400
F	0.24215700	-4.34022300	0.00867500
F	-0.27485200	-4.41344900	2.12112500
F	1.81412700	-4.38177200	1.51449300
C	-0.82538800	5.85407600	-0.49022500
C	-0.11067800	6.82743600	0.22938800
C	-1.41088300	6.25215600	-1.70099100
C	-0.00585900	8.14243000	-0.22197000
H	0.38952900	6.56265700	1.15749300
C	-1.30857000	7.56778700	-2.15836600
H	-1.97630200	5.54288800	-2.29238200
C	-0.60924400	8.52145700	-1.42123500
H	0.55303500	8.86739600	0.36368300
H	-1.78363500	7.84320400	-3.09620200
H	-0.53230600	9.54527800	-1.77657200
C	-1.81882300	3.48594700	-0.81367200
H	-1.67814700	2.44556500	-0.49894300
H	-1.49205600	3.47385000	-1.86479600
C	-3.31560600	3.74527300	-0.80120300
C	-3.94086600	4.76128300	-0.19519400
H	-5.02339400	4.84925300	-0.23583400
H	-3.41956500	5.54382400	0.34544300
C	-0.88426200	1.91211700	2.51277400
H	-0.12972800	1.23522100	2.92341800
H	-1.74055500	1.90264500	3.20613100
H	-1.25038500	1.50810400	1.56726300
C	-4.09081900	2.70511200	-1.57785700
H	-3.92241000	1.70122900	-1.17023100
H	-5.16484100	2.91121100	-1.56019100
H	-3.76410600	2.67785200	-2.62702200

TS-EF-5S-3

l imaginary frequency

H = -5315.358983

G = -5315.559771

E(M06-2X-DCM) = -5316.242884

O	-1.06108500	-2.54815200	-0.68477300
O	-2.87756900	-0.93751400	0.24618100
P	-1.26811200	-1.05045900	-0.04877600
O	-0.92490700	0.04712100	-1.01259700
C	-2.86319900	-3.29615500	-4.38706600
C	-3.58787100	-3.41230800	-3.20507700

C	-2.95495400	-3.24494900	-1.96534600
C	-0.85057700	-2.75262200	-3.09882600
C	-1.50016700	-3.00587000	-4.32030800
C	-3.50703900	-1.86242700	1.08393900
C	-3.84627200	-3.12233300	0.58618600
C	-4.32784800	-4.09937700	1.47350000
C	-4.56892000	-3.79599300	2.80826700
C	-4.34602500	-2.49440300	3.25408400
C	-3.81126100	-1.50482800	2.41358200
H	-0.91647300	-2.94976800	-5.23446100
H	-4.57524000	-2.22643600	4.28135900
C	-3.89276900	-3.66592800	-0.84158200
C	-5.27606200	-3.37843500	-1.51795700
H	-5.50632600	-2.31249000	-1.40719000
H	-6.09195400	-3.94617700	-1.05981200
H	-5.57389000	-5.63866000	0.59159200
H	-4.11106400	-6.26571600	1.34422300
C	-1.62288600	-2.84283900	-1.92427400
H	-3.34320400	-3.43991300	-5.35188000
H	-4.94122100	-4.55359200	3.49319900
C	-5.05886600	-3.71258800	-3.01139200
H	-5.69905500	-3.11871100	-3.67388500
H	-5.28164200	-4.76791800	-3.22243800
C	-4.51009000	-5.42418200	0.76648100
C	-3.75513700	-5.20044100	-0.55941200
H	-2.69353300	-5.43721600	-0.42456600
H	-4.13154700	-5.81176200	-1.38545100
C	-3.68454700	-0.11290200	2.95494000
C	-2.72132000	0.18910100	3.94638800
C	-4.63779000	0.86260800	2.56782300
C	-1.74447900	-0.75969600	4.38672200
C	-2.70297300	1.50357100	4.55014200
C	-4.59874400	2.17814800	3.16676200
C	-0.82763800	-0.44100900	5.35269600
H	-1.71471400	-1.73306600	3.91588700
C	-1.73426500	1.79224300	5.56277500
C	-3.63254000	2.46308000	4.13707700
C	-0.82445900	0.84859200	5.95628200
H	-0.07926100	-1.17183100	5.64303800
H	-1.74006000	2.78213100	6.01388600
H	-3.62121600	3.44794100	4.60119700
H	-0.09037300	1.08089000	6.72316500
C	0.61168500	-2.43767500	-3.09213100
C	1.08800100	-1.28363500	-3.76462800

C	1. 52790900	-3. 33338400	-2. 48522400
C	0. 21795900	-0. 32803100	-4. 38441300
C	2. 51082100	-1. 03641500	-3. 84312900
C	2. 94463500	-3. 05062600	-2. 53450400
C	0. 71352300	0. 74932600	-5. 07454800
H	-0. 85317800	-0. 46666700	-4. 30034700
C	2. 98545500	0. 10584200	-4. 56212400
C	3. 39791000	-1. 91983900	-3. 22060800
C	2. 11757000	0. 97039900	-5. 17286000
H	0. 02714900	1. 44312800	-5. 55426400
H	4. 05953100	0. 26722500	-4. 61804300
H	4. 46815400	-1. 72974400	-3. 27862800
H	2. 49322000	1. 82664800	-5. 72673600
C	-6. 61563600	1. 54875500	1. 30224100
H	-7. 40896100	1. 31050200	0. 59854100
C	-5. 68891400	0. 59380400	1. 63244500
H	-5. 75549800	-0. 39427700	1. 19134500
C	-6. 55538700	2. 85052000	1. 87593100
H	-7. 29636300	3. 59618500	1. 60036600
C	-5. 57338600	3. 15124400	2. 78079800
H	-5. 52488100	4. 13656900	3. 23929600
C	2. 03129200	-5. 37670800	-1. 24344500
H	1. 69057200	-6. 28388100	-0. 75176900
C	3. 42123500	-5. 07076600	-1. 26207500
H	4. 12673800	-5. 73820100	-0. 77499100
C	3. 86322300	-3. 94205800	-1. 89612600
H	4. 92094100	-3. 69399300	-1. 91642500
C	1. 12057000	-4. 54114900	-1. 83422600
H	0. 06795700	-4. 79703400	-1. 81303100
C	-1. 13867600	3. 64256600	-1. 77771500
C	-1. 38833900	3. 38910800	-0. 26883300
H	-2. 36143800	3. 81424800	0. 01879900
H	-1. 52452100	2. 31201000	-0. 13024500
C	-0. 38376400	3. 85723500	0. 74717100
C	0. 31558100	3. 16879000	-2. 15350500
H	0. 99287300	4. 01827200	-2. 20779100
H	0. 29629400	2. 69877500	-3. 14250600
N	0. 91705100	2. 19619200	-1. 23438900
C	2. 17583700	2. 27031200	-0. 76282300
N	2. 72874500	1. 13491100	-0. 30537900
C	4. 00490100	0. 94975800	0. 30117500
C	4. 45190900	1. 70324800	1. 38828500
C	4. 78255000	-0. 09966200	-0. 18948000
C	5. 70029000	1. 42654300	1. 94443800

C	6.02259100	-0.37577100	0.38540400
H	4.40956100	-0.69716400	-1.01317600
C	6.49454200	0.39068200	1.44905300
H	7.46039700	0.18038600	1.89248500
C	6.82306200	-1.54288700	-0.12967900
C	6.21998800	2.28637100	3.06722400
F	6.40839800	-2.71288500	0.40243100
F	8.13679100	-1.41881200	0.15146500
F	6.70765100	-1.66951100	-1.47702500
F	6.95693400	3.32019200	2.59791900
F	7.01531200	1.58714400	3.90545500
F	5.21853700	2.81779700	3.80040100
S	3.01534900	3.79356600	-0.68594400
H	3.83258700	2.48574100	1.80380400
H	2.19849800	0.25340000	-0.37646300
H	0.41924200	1.29166700	-1.16689400
C	0.46995500	4.94625100	0.57123600
H	0.23275700	5.67586500	-0.20050600
H	1.56928600	4.43512400	0.01879800
H	0.92815100	5.36046500	1.47052200
N	-0.56851800	-1.10438300	1.40528400
S	0.99280300	-1.27203900	1.61016800
O	1.51580800	-0.34913100	2.62598600
O	1.76512200	-1.38402200	0.34001900
C	1.15676100	-2.97289000	2.36687800
F	0.50424300	-3.02690600	3.53936000
F	2.44774600	-3.23949900	2.58603100
F	0.64953700	-3.90012200	1.55157900
C	-1.31759500	5.10593200	-2.22274300
C	-0.82361400	5.51482100	-3.47450200
C	-2.01710500	6.05867000	-1.46620800
C	-1.01124300	6.81392900	-3.94488200
H	-0.28860900	4.80857500	-4.10315400
C	-2.20819600	7.36158600	-1.93304700
H	-2.42665200	5.79539900	-0.49669500
C	-1.70617900	7.74739200	-3.17492900
H	-0.61370400	7.09449800	-4.91661600
H	-2.75328400	8.07354900	-1.31888300
H	-1.85383100	8.76050400	-3.53819300
C	-2.14121300	2.73446200	-2.59371400
H	-1.89457300	2.87337300	-3.65485500
H	-1.90620900	1.69614800	-2.33942400
C	-3.62868900	2.96926000	-2.39857200
C	-4.32420100	2.23569100	-1.52067800

H	-3.86238300	1.45714600	-0.91974100
H	-5.39214400	2.38143100	-1.37979000
C	-4.31021700	3.98596100	-3.28599300
H	-4.18042900	3.71920900	-4.34449300
H	-5.38465300	4.03180000	-3.08102100
H	-3.89615000	4.99257500	-3.16591000
C	-0.32945800	3.06423100	2.01297400
H	-0.02689600	2.02479800	1.82757400
H	0.34604400	3.49985900	2.75293000
H	-1.33529000	2.99510000	2.45074500

TS-EF-5S-4

l imaginary frequency

H = -5315.357088

G = -5315.558341

E(M06-2X-DCM) = -5316.242190

O	-1.09458900	-2.52706000	-0.66947000
O	-2.90646700	-0.89297300	0.22811500
P	-1.29598600	-1.01997500	-0.05324500
O	-0.93448400	0.06387900	-1.02601400
C	-2.88456500	-3.31152300	-4.36992000
C	-3.61522600	-3.40853100	-3.18979300
C	-2.98688900	-3.22865500	-1.94948500
C	-0.87379900	-2.76615100	-3.07931200
C	-1.51979900	-3.02998700	-4.30051300
C	-3.54632900	-1.80145600	1.07578900
C	-3.88842500	-3.06733700	0.59562500
C	-4.37834000	-4.02923400	1.49475700
C	-4.62513500	-3.70493900	2.82357400
C	-4.40112700	-2.39706100	3.25034900
C	-3.85868700	-1.42225200	2.39770900
H	-0.93151000	-2.99035500	-5.21256900
H	-4.63623800	-2.11225800	4.27177500
C	-3.93113800	-3.63087500	-0.82432400
C	-5.31058200	-3.34744500	-1.51034900
H	-5.53846600	-2.27954500	-1.41329700
H	-6.13025100	-3.90686700	-1.04876700
H	-5.62592800	-5.57712600	0.63015700
H	-4.16819200	-6.19794300	1.39757700
C	-1.65240100	-2.83441700	-1.90745100
H	-3.36102900	-3.46465600	-5.33503500
H	-5.00342400	-4.45077800	3.51804800
C	-5.08825500	-3.70057000	-2.99866400
H	-5.72369200	-3.11298500	-3.67130000

H	-5.31391900	-4.75764000	-3.19748100
C	-4.56212900	-5.36356000	0.80614500
C	-3.80105800	-5.16176900	-0.51996200
H	-2.74099600	-5.40101400	-0.37760900
H	-4.17689400	-5.78322900	-1.33867900
C	-3.73571400	-0.02082300	2.91517900
C	-2.77122900	0.30410500	3.89775900
C	-4.69473600	0.94302600	2.51290300
C	-1.79471000	-0.63478100	4.35938900
C	-2.75246800	1.63220400	4.47131800
C	-4.65531000	2.27209200	3.08136500
C	-0.87682700	-0.29424200	5.31680900
H	-1.76707600	-1.61931300	3.91236100
C	-1.78178200	1.94418200	5.47532100
C	-3.68402400	2.58129200	4.03916900
C	-0.87181900	1.00949000	5.88942000
H	-0.12914900	-1.01884100	5.62392400
H	-1.78706300	2.94406600	5.90384700
H	-3.67188200	3.57672600	4.48011400
H	-0.13684800	1.25916600	6.64997700
C	0.59169300	-2.46664700	-3.06884000
C	1.08469300	-1.32741400	-3.75436300
C	1.49431600	-3.36439300	-2.44467500
C	0.22905300	-0.37096000	-4.39253700
C	2.51062500	-1.09702900	-3.82769400
C	2.91448600	-3.09877300	-2.49052900
C	0.74034000	0.69172700	-5.09385600
H	-0.84404200	-0.49704400	-4.31395600
C	3.00203200	0.03023500	-4.55894600
C	3.38421700	-1.98209800	-3.18863200
C	2.14733800	0.89598900	-5.18642600
H	0.06440000	1.38664600	-5.58645400
H	4.07813400	0.17901800	-4.61061500
H	4.45688300	-1.80498600	-3.24339200
H	2.53569200	1.74048100	-5.74951100
C	-6.68474500	1.59359500	1.24740200
H	-7.48216500	1.33722100	0.55492300
C	-5.75213600	0.64956900	1.59193500
H	-5.81779600	-0.34823200	1.17327000
C	-6.62370000	2.90863300	1.78981300
H	-7.36878800	3.64567200	1.50245500
C	-5.63516000	3.23357100	2.67925800
H	-5.58605600	4.22957100	3.11398800
C	1.96778400	-5.39640500	-1.17271400

H	1. 61403100	-6. 29274800	-0. 67049300
C	3. 36134200	-5. 10737200	-1. 18917000
H	4. 05674300	-5. 77660500	-0. 69018600
C	3. 81953000	-3. 99263500	-1. 83628800
H	4. 88031800	-3. 75812600	-1. 85579700
C	1. 06981500	-4. 55834200	-1. 77924500
H	0. 01426300	-4. 80187400	-1. 75988500
C	-1. 04875400	3. 64718000	-1. 82814400
C	-1. 31676800	3. 41871300	-0. 31744800
H	-2. 26957000	3. 89142300	-0. 03710200
H	-1. 48529800	2. 34843600	-0. 16338700
C	-0. 30478700	3. 87737200	0. 69703000
C	0. 39732400	3. 13461700	-2. 18161000
H	1. 09410700	3. 96712000	-2. 24582600
H	0. 37632600	2. 64530200	-3. 16115400
N	0. 97066900	2. 16938100	-1. 23690300
C	2. 23112600	2. 22760000	-0. 76427300
N	2. 76186100	1. 08935500	-0. 28855600
C	4. 03260600	0. 89064000	0. 32459200
C	4. 48978500	1. 65245000	1. 40172800
C	4. 79333700	-0. 17911900	-0. 14830900
C	5. 73154800	1. 36241300	1. 96572800
C	6. 02715900	-0. 46765100	0. 43398200
H	4. 41250900	-0. 78189800	-0. 96458600
C	6. 50928500	0. 30597800	1. 48775600
H	7. 47028000	0. 08579300	1. 93687400
C	6. 80944400	-1. 65459900	-0. 06345000
C	6. 26276200	2. 22947300	3. 07755300
F	6. 36827000	-2. 81135300	0. 47621400
F	8. 12299800	-1. 55277500	0. 22683000
F	6. 70189200	-1. 79161500	-1. 41045900
F	7. 01780900	3. 24413100	2. 59566900
F	7. 04418900	1. 52909200	3. 92778300
F	5. 26832000	2. 78767700	3. 80040000
S	3. 09774800	3. 73558400	-0. 71043400
H	3. 88311700	2. 45188500	1. 80347700
H	2. 21627200	0. 21621800	-0. 34972900
H	0. 45695800	1. 27457600	-1. 16212600
C	0. 56196300	4. 95447300	0. 50781200
H	0. 33081300	5. 67509700	-0. 27459800
H	1. 65055300	4. 42141500	-0. 02732900
H	1. 02013500	5. 37732900	1. 40316100
N	-0. 60731500	-1. 06262700	1. 40674300
S	0. 94874800	-1. 25147500	1. 62745600

O	1.47878600	-0.31889100	2.63113200
O	1.73034800	-1.39794200	0.36634100
C	1.08019600	-2.94093300	2.41516500
F	0.41702800	-2.96410100	3.58277300
F	2.36493400	-3.22332900	2.65024400
F	0.56558200	-3.87431300	1.61168000
C	-1.19506000	5.10918300	-2.29233100
C	-0.61780300	5.51407500	-3.50944600
C	-1.95584200	6.06081000	-1.59706800
C	-0.77545100	6.81061600	-3.99827500
H	-0.03874200	4.80816400	-4.09798200
C	-2.11372900	7.36201100	-2.07971600
H	-2.43895300	5.80073800	-0.66141300
C	-1.52348300	7.74579000	-3.28234600
H	-0.31107100	7.08751600	-4.94100600
H	-2.70618100	8.07328800	-1.51030100
H	-1.64627500	8.75756900	-3.65850600
C	-2.06052100	2.76517100	-2.66169700
H	-1.80901200	2.93395900	-3.71500800
H	-1.83570600	1.71659900	-2.43730300
C	-3.54712800	3.01397100	-2.46856200
C	-4.19678600	3.93634800	-3.18909600
H	-3.69051400	4.55811600	-3.92260100
H	-5.26521100	4.10099500	-3.06976400
C	-4.27638300	2.12546700	-1.48990600
H	-3.90421900	2.22738000	-0.46437800
H	-5.34787800	2.34454800	-1.47407200
H	-4.14085900	1.06741400	-1.74757400
C	-0.26515100	3.09934200	1.97195300
H	0.01765800	2.05197500	1.80052000
H	0.41782500	3.53193300	2.70674600
H	-1.27221500	3.05443800	2.41030600

TS-EF-5S-5

l imaginary frequency

H = -5315.360231

G = -5315.558841

E(M06-2X-DCM) = -5316.247651

O	-0.64092400	-2.71942000	-0.52705300
O	-2.76702800	-1.23189300	-0.39471600
P	-1.13878800	-1.19236100	-0.20846700
O	-0.61629500	-0.18730900	-1.18807200
C	-1.23737000	-4.05567900	-4.45098500
C	-2.25541900	-4.14003500	-3.50673400

C	-2.02161600	-3.76807100	-2.17519800
C	0.26870300	-3.14261200	-2.74561400
C	0.01721800	-3.59340100	-4.05423600
C	-3.54237800	-2.11451300	0.35862800
C	-3.62743000	-3.45476700	-0.02242600
C	-4.27619000	-4.36607600	0.82677000
C	-4.92569400	-3.93156500	1.97651300
C	-4.93640200	-2.56950400	2.27123300
C	-4.24483200	-1.63490200	1.48230700
H	0.82901100	-3.55394000	-4.77442600
H	-5.47661800	-2.20862800	3.14148000
C	-3.20936700	-4.16652700	-1.30811300
C	-4.35529200	-4.12469800	-2.37577200
H	-4.69471100	-3.08819100	-2.48660700
H	-5.22008200	-4.72952900	-2.08563200
H	-5.08208800	-6.13668200	-0.13016300
H	-3.86319900	-6.49109000	1.08951700
C	-0.79469300	-3.20945900	-1.82516700
H	-1.40764600	-4.35336300	-5.48264800
H	-5.43093100	-4.63698600	2.63129200
C	-3.68717500	-4.59636100	-3.68643300
H	-4.15701800	-4.16612200	-4.57837200
H	-3.74701900	-5.68833600	-3.79584000
C	-4.13758800	-5.77865200	0.30319900
C	-3.04348100	-5.62919000	-0.77421300
H	-2.05402700	-5.72331200	-0.31239100
H	-3.11199900	-6.37478400	-1.57235700
C	-4.36172500	-0.18641900	1.84631000
C	-3.82680200	0.28175900	3.07158700
C	-5.13704200	0.67976700	1.03392600
C	-2.99448700	-0.52911000	3.90802300
C	-4.10731100	1.63151500	3.50884500
C	-5.39135700	2.03476600	1.47242300
C	-2.49723400	-0.05553100	5.09334300
H	-2.72442500	-1.52030100	3.56914700
C	-3.58773400	2.07979400	4.76541300
C	-4.88020000	2.46986600	2.69956600
C	-2.80793100	1.26083600	5.53828200
H	-1.84182600	-0.68362700	5.68891400
H	-3.82977900	3.08876500	5.09282200
H	-5.10349700	3.47981300	3.04001400
H	-2.41574200	1.61406300	6.48825600
C	1.64163400	-2.65982200	-2.39753700
C	2.18052200	-1.53205900	-3.06598400

C	2. 44136100	-3. 39083400	-1. 48329600
C	1. 41445600	-0. 71934900	-3. 96443300
C	3. 55929100	-1. 15887900	-2. 84354800
C	3. 80415000	-2. 97617600	-1. 23684700
C	1. 97628500	0. 34322100	-4. 62448900
H	0. 36578800	-0. 94942300	-4. 10850200
C	4. 11272900	-0. 05316400	-3. 56538700
C	4. 33032400	-1. 88324900	-1. 93092000
C	3. 34831900	0. 67689100	-4. 43552800
H	1. 36918800	0. 93908000	-5. 30124300
H	5. 16021800	0. 18964400	-3. 40405800
H	5. 36240400	-1. 58587800	-1. 75708200
H	3. 78078400	1. 51195400	-4. 98022200
C	-6. 47441800	1. 12547300	-0. 96603600
H	-6. 90164900	0. 78360000	-1. 90459500
C	-5. 72327900	0. 26695100	-0. 20612700
H	-5. 56825300	-0. 75091100	-0. 54399000
C	-6. 70838500	2. 46263100	-0. 53643300
H	-7. 31079100	3. 12794700	-1. 14881500
C	-6. 18535200	2. 89785100	0. 65191700
H	-6. 37626200	3. 90947200	1. 00424800
C	2. 77111600	-5. 23527500	0. 08653500
H	2. 38495200	-6. 11411100	0. 59602000
C	4. 10286500	-4. 80484900	0. 34571600
H	4. 71853500	-5. 35241600	1. 05408600
C	4. 60215300	-3. 70955600	-0. 30439200
H	5. 62095900	-3. 37405200	-0. 12594000
C	1. 97382800	-4. 55716300	-0. 79767400
H	0. 96667900	-4. 90935600	-0. 98681200
C	-1. 62940300	3. 53769900	-1. 07155300
C	-1. 67250900	3. 21321900	0. 45383800
H	-2. 65925200	3. 49212300	0. 85727400
H	-1. 63998000	2. 12781400	0. 59940200
C	-0. 69090700	3. 82852600	1. 39704200
C	-0. 17410500	3. 33929900	-1. 60821800
H	0. 39548800	4. 26253700	-1. 53764400
H	-0. 21699300	3. 07392700	-2. 66936600
N	0. 60609200	2. 32592500	-0. 90003900
C	1. 87980500	2. 49310100	-0. 48346100
N	2. 51439400	1. 38440100	-0. 04775500
C	3. 85767800	1. 32600900	0. 42660300
C	4. 10366800	0. 93883900	1. 74792000
C	4. 91547300	1. 56201500	-0. 44727400
C	5. 42015600	0. 79694300	2. 18222800

C	6. 22924500	1. 40321200	-0. 00193700
H	4. 70969400	1. 83839800	-1. 47449600
C	6. 48980500	1. 02312700	1. 31175900
H	7. 51093700	0. 89882300	1. 65373600
C	7. 34428500	1. 55768500	-0. 99913700
C	5. 72761900	0. 39197200	3. 60058800
F	7. 35714600	0. 51700500	-1. 87838300
F	8. 55811300	1. 59412200	-0. 41518000
F	7. 20796500	2. 67842200	-1. 73813800
F	6. 47926300	1. 33076000	4. 22370400
F	6. 43978800	-0. 75798000	3. 63929600
F	4. 61624700	0. 20848200	4. 33652300
S	2. 64314900	4. 04502600	-0. 40722900
H	3. 27369300	0. 74488000	2. 41689200
H	1. 99631000	0. 50387800	0. 05877200
H	0. 24620100	1. 35791900	-0. 96889800
C	0. 03474800	5. 01294200	1. 11260300
H	-0. 39175500	5. 67586200	0. 35959400
H	1. 04284100	4. 62656300	0. 56196500
H	0. 43527000	5. 53262600	1. 98522600
N	-0. 90195300	-0. 97455800	1. 37992400
S	0. 53543700	-0. 97519700	2. 04329300
O	0. 65506000	0. 07102200	3. 07628700
O	1. 66209800	-1. 08623900	1. 08161800
C	0. 59324200	-2. 57890300	3. 00290000
F	-0. 38138300	-2. 60050700	3. 92635600
F	1. 77142900	-2. 68398200	3. 62301000
F	0. 43228200	-3. 61943500	2. 18377100
C	-2. 12587000	4. 96991100	-1. 37087600
C	-1. 49342500	5. 81355900	-2. 29813900
C	-3. 29857500	5. 45285500	-0. 76258200
C	-1. 98763600	7. 09026200	-2. 57846800
H	-0. 60935800	5. 48399600	-2. 83170300
C	-3. 79593800	6. 72534000	-1. 03995400
H	-3. 85757500	4. 82350800	-0. 07595100
C	-3. 13756900	7. 55750600	-1. 94671100
H	-1. 46851300	7. 71417500	-3. 30104200
H	-4. 70347100	7. 06419200	-0. 54696800
H	-3. 52151800	8. 55059500	-2. 16272700
C	-2. 62675800	2. 51004900	-1. 73836800
H	-2. 34376900	1. 50718100	-1. 40582900
H	-3. 62074900	2. 71072400	-1. 32440900
C	-2. 70662100	2. 50747200	-3. 25990100
C	-3. 40013200	3. 42706400	-3. 94175700

H	-3.93386600	4.23486200	-3.45034300
H	-3.46295100	3.39567700	-5.02724700
C	-2.03222900	1.35371000	-3.96601700
H	-2.47857700	0.40115300	-3.65202100
H	-2.12773000	1.43972700	-5.05349300
H	-0.96830300	1.27105500	-3.71408200
C	-0.47516500	3.12061400	2.68222000
H	-0.02399800	2.12719100	2.52504300
H	0.14889100	3.68843500	3.37561300
H	-1.44204300	2.89796500	3.15639600

TS-EF-5S-6

l imaginary frequency

H = -5315.355636

G = -5315.553336

E(M06-2X-DCM) = -5316.237463

O	0.83954900	-2.85798200	-0.07365000
O	2.59674000	-1.02469100	-0.55958900
P	1.00023100	-1.23514800	-0.28078100
O	0.63436900	-0.45313200	0.93774300
C	3.05787000	-4.66006100	2.99269100
C	3.61352700	-4.46078800	1.73363500
C	2.85086200	-3.91214800	0.69148400
C	0.95205100	-3.68964700	2.20892100
C	1.73001500	-4.29637500	3.20998000
C	3.17614200	-1.56962100	-1.70569700
C	3.50675200	-2.92282600	-1.73362100
C	3.89850200	-3.50518600	-2.94919000
C	4.08963400	-2.72053600	-4.08153200
C	3.89637300	-1.34135500	-3.99052100
C	3.42421800	-0.73607800	-2.81430600
H	1.27682400	-4.46164900	4.18308600
H	4.09164000	-0.71017800	-4.85251200
C	3.64314100	-3.94794800	-0.61130700
C	5.10519200	-3.93565000	-0.04309800
H	5.38601100	-2.89943200	0.17797500
H	5.83370400	-4.33333000	-0.75626600
H	5.10763100	-5.30345600	-2.80725500
H	3.55820100	-5.55842900	-3.60178900
C	1.54910300	-3.48364000	0.94979400
H	3.64585700	-5.09057200	3.79935800
H	4.40203900	-3.16692600	-5.02235300
C	5.02564400	-4.74043700	1.27035700
H	5.77883000	-4.43090100	2.00387000

H	5.18078100	-5.81413900	1.09249100
C	4.05021200	-5.00409800	-2.79421800
C	3.40602000	-5.26915300	-1.41402600
H	2.32693900	-5.42156400	-1.53043600
H	3.81585900	-6.14740600	-0.90493200
C	3.26346500	0.75015800	-2.75482900
C	2.33421700	1.40687400	-3.59878000
C	4.11417200	1.50875200	-1.90975600
C	1.43755200	0.70118900	-4.46465200
C	2.26224800	2.85157100	-3.59502900
C	4.00395200	2.94968400	-1.89091400
C	0.57817900	1.36702100	-5.29828000
H	1.42423200	-0.38106100	-4.43147200
C	1.35166400	3.50819800	-4.48204500
C	3.08306400	3.58096800	-2.73145100
C	0.54161900	2.79036800	-5.32099600
H	-0.09876500	0.80339700	-5.93368100
H	1.32975800	4.59605800	-4.48166600
H	3.01058700	4.66633400	-2.71642900
H	-0.13508300	3.30136400	-6.00178800
C	-0.46466700	-3.32711500	2.52863700
C	-0.73318900	-2.32289600	3.49082300
C	-1.52892300	-4.06897500	1.95991700
C	0.29632900	-1.52686600	4.09190800
C	-2.09673600	-2.06985000	3.89890100
C	-2.88817000	-3.79727900	2.36906500
C	0.00664400	-0.58504200	5.04612000
H	1.32138400	-1.66399700	3.76897400
C	-2.35634900	-1.07522500	4.89415900
C	-3.13487900	-2.80882700	3.32563100
C	-1.33780700	-0.35766000	5.45960800
H	0.80742300	0.00720500	5.47983000
H	-3.38815800	-0.90593700	5.19421500
H	-4.15886100	-2.62200900	3.64437200
H	-1.54785100	0.39196400	6.21783600
C	5.92183600	1.67721400	-0.26993700
H	6.67437800	1.19620800	0.34931100
C	5.11799200	0.91596200	-1.07753300
H	5.24676000	-0.15979900	-1.09711400
C	5.78450300	3.09344400	-0.23287900
H	6.42511600	3.68150000	0.41891500
C	4.85361700	3.70813100	-1.02559200
H	4.74086400	4.78825800	-1.01160600
C	-2.36927300	-5.83640400	0.49392600

H	-2.18018300	-6.62708100	-0.22703100
C	-3.70681800	-5.56066500	0.89643300
H	-4.52500100	-6.14550300	0.48433800
C	-3.95396400	-4.57078800	1.80987200
H	-4.96905300	-4.36124700	2.14057500
C	-1.32137400	-5.12055100	1.01050800
H	-0.30910400	-5.35225700	0.70036400
N	0.27623200	-0.94129400	-1.70460100
S	-1.27835300	-0.83410800	-1.90026800
O	-1.64547700	0.16481100	-2.92152300
O	-2.06363700	-0.77901500	-0.63288000
C	-1.77809100	-2.46162000	-2.67166400
F	-1.10881700	-2.64300500	-3.81644700
F	-3.08996500	-2.44893000	-2.93691500
F	-1.51075600	-3.47476100	-1.84524500
C	-5.13969500	1.78806900	-0.68363400
C	-4.33831300	2.32673100	-1.93196100
H	-5.07783400	2.63090100	-2.69065000
H	-3.79005500	1.48965900	-2.37253100
C	-3.38221800	3.48103300	-1.81716400
C	-4.27400500	1.88040200	0.60792600
H	-4.43642300	2.84608300	1.08151900
H	-4.61500300	1.13396400	1.33149100
N	-2.82606800	1.73541800	0.41879400
C	-1.89384600	2.48435400	1.05310700
N	-0.65125300	1.97591200	1.13991900
C	0.50563700	2.64859800	1.63461700
C	0.94501300	3.86164400	1.10046000
C	1.25187100	2.01065300	2.62552900
C	2.10923600	4.44959100	1.59311000
C	2.42185400	2.60409000	3.10032400
H	0.92530300	1.04918400	3.00228500
C	2.85472900	3.82863900	2.59662500
H	3.76771700	4.28171100	2.96180200
C	3.18372700	1.90939400	4.19788800
C	2.53699000	5.78758900	1.05342700
F	2.54121400	2.01821700	5.39011900
F	3.31844000	0.58757000	3.95682900
F	4.41927700	2.42354700	4.36810500
F	1.88914300	6.80583200	1.66407400
F	3.86013700	6.00615000	1.22172900
F	2.27465600	5.90278300	-0.27183500
S	-2.27497000	4.06224400	1.67123900
H	0.39313300	4.33666600	0.30001300

H	-0.47398600	0.96938300	0.95664100
H	-2.50807400	0.83097300	0.03082600
C	-3.59757300	4.63560700	-1.04669600
H	-4.61377300	4.87064500	-0.73700400
H	-3.06254900	4.38714500	0.08065900
H	-3.01221500	5.51181600	-1.33211400
C	-6.42587300	2.66109700	-0.43516300
H	-7.08076400	2.55285600	-1.30808700
H	-6.12764400	3.71272700	-0.40555100
C	-5.56232600	0.34899300	-1.06050900
C	-5.12794700	-0.79150500	-0.37347500
C	-6.40601100	0.15474600	-2.16972600
C	-5.53048500	-2.07088800	-0.76669800
H	-4.44470200	-0.71622500	0.46327800
C	-6.81401100	-1.11773300	-2.56259000
H	-6.75492800	1.00706600	-2.74700200
C	-6.37979600	-2.24067400	-1.85691700
H	-5.15457400	-2.93262500	-0.22316000
H	-7.46763200	-1.22955100	-3.42371400
H	-6.68936900	-3.23601400	-2.16342100
C	-7.23073200	2.37690700	0.82338000
C	-7.21380500	3.24418600	1.84336200
H	-6.61952000	4.15477700	1.81956400
H	-7.79979300	3.07709400	2.74364100
C	-2.14153500	3.37988900	-2.63827700
H	-2.42751800	3.45220200	-3.70016000
H	-1.43096600	4.18400300	-2.43139500
H	-1.66306900	2.39840000	-2.54691400
C	-8.09313000	1.13726500	0.86671500
H	-7.49692800	0.21918300	0.83461500
H	-8.70421200	1.11852100	1.77436800
H	-8.76535500	1.09689000	-0.00035400

TS-EF-5S-7

l imaginary frequency

H = -5315.344227

G = -5315.546295

E(M06-2X-DCM) = -5316.232582

O	2.68528000	-1.50272000	0.87493600
O	2.05608000	-0.68020000	-1.49490500
P	1.47337600	-0.79050200	0.03738900
O	1.15580900	0.61183300	0.46940400
C	6.46760700	0.28214000	1.06960600
C	6.09902000	-0.47961100	-0.03419700

C	4. 86036300	-1. 13878900	-0. 06820000
C	4. 30224000	-0. 18793800	2. 11213700
C	5. 58358300	0. 39075000	2. 14177600
C	2. 34204100	-1. 83456100	-2. 22423400
C	3. 54619600	-2. 50247000	-2. 00672200
C	3. 75053400	-3. 75459400	-2. 60898400
C	2. 83002100	-4. 26489500	-3. 51733600
C	1. 69379600	-3. 51589300	-3. 82180100
C	1. 41163900	-2. 30117200	-3. 17503100
H	5. 87343900	0. 95312000	3. 02427000
H	0. 98468000	-3. 88454800	-4. 55697800
C	4. 81394200	-2. 08370200	-1. 26576400
C	5. 80519500	-1. 34991900	-2. 23280200
H	5. 26365600	-0. 54970300	-2. 75176400
H	6. 21707400	-2. 01785700	-2. 99536800
H	5. 81955600	-4. 35535900	-2. 87965100
H	4. 90308900	-5. 43508500	-1. 83477400
C	3. 94842000	-0. 92712400	0. 96572700
H	7. 43438800	0. 77810200	1. 10638200
H	2. 99231200	-5. 22902700	-3. 99259100
C	6. 87749200	-0. 74032800	-1. 30521800
H	7. 32746300	0. 17027900	-1. 71760500
H	7. 70223900	-1. 44538200	-1. 13035500
C	5. 03438700	-4. 38266000	-2. 11107000
C	5. 39589200	-3. 49131800	-0. 90296500
H	4. 88808200	-3. 86005300	-0. 00449800
H	6. 46916900	-3. 45866100	-0. 69123200
C	0. 17176800	-1. 55010100	-3. 54616600
C	-1. 10166800	-2. 13220800	-3. 32672500
C	0. 27445800	-0. 29895900	-4. 20606200
C	-1. 27617500	-3. 37426500	-2. 63557400
C	-2. 29060900	-1. 45339400	-3. 79319700
C	-0. 92587300	0. 38763100	-4. 62981000
C	-2. 51801100	-3. 92425200	-2. 45846700
H	-0. 40806700	-3. 86231500	-2. 21304000
C	-3. 56854500	-2. 06719600	-3. 59627200
C	-2. 17204500	-0. 20991600	-4. 41921900
C	-3. 68215100	-3. 27368300	-2. 95752800
H	-2. 61962200	-4. 85392500	-1. 90674300
H	-4. 45276400	-1. 54889400	-3. 96026600
H	-3. 07019700	0. 30158600	-4. 76001200
H	-4. 65920000	-3. 72062500	-2. 80205200
C	3. 39829700	-0. 02282900	3. 29151200
C	3. 01693800	1. 27887800	3. 70522600

C	2.99838600	-1.15282200	4.04892900
C	3.36015200	2.46306400	2.97369300
C	2.24342100	1.44701900	4.91511800
C	2.18201100	-0.97037800	5.22731400
C	3.02743100	3.71217800	3.43293000
H	3.88720200	2.36376500	2.03219000
C	1.91462600	2.76718400	5.35910100
C	1.83646100	0.32043200	5.63340200
C	2.30533100	3.87289500	4.65030600
H	3.31231200	4.58820700	2.85595100
H	1.35253000	2.87142400	6.28465800
H	1.24256800	0.45121700	6.53586000
H	2.06304400	4.87024300	5.00872900
C	1.59545400	1.53706000	-5.14136600
H	2.56339800	1.98106300	-5.35762700
C	1.52943600	0.32211400	-4.50904800
H	2.44496800	-0.19157000	-4.23924100
C	0.40805100	2.22293500	-5.52566000
H	0.47844600	3.18606100	-6.02366700
C	-0.81421700	1.65756600	-5.27924600
H	-1.72935800	2.16182800	-5.58073000
C	2.97674600	-3.56036200	4.47001600
H	3.28691700	-4.56404900	4.19219500
C	2.14392000	-3.37566200	5.60939200
H	1.81836700	-4.23792300	6.18480500
C	1.76578700	-2.11402700	5.97753900
H	1.13982400	-1.95414900	6.85215900
C	3.39214700	-2.48994900	3.72303200
H	4.03545500	-2.65503500	2.86728400
N	0.29921000	-1.88986100	-0.02092200
S	-0.66200400	-2.21880700	1.19828000
O	-2.07621800	-2.06184200	0.77485900
O	-0.28894900	-1.64693700	2.50105800
C	-0.44732600	-4.06295400	1.39225900
F	-0.74127100	-4.71103000	0.25585800
F	-1.26248500	-4.50227500	2.35680200
F	0.81587700	-4.33973400	1.72890100
C	0.35919000	4.06460400	-0.70587000
C	0.34970000	3.94287800	0.86804200
H	0.78799600	4.87160400	1.25976100
H	1.04820600	3.14445300	1.12605300
C	-0.92536800	3.70219100	1.63735900
C	-0.48607400	2.91887900	-1.37659900
H	-1.27940300	3.36667600	-1.97150800

H	0.12712400	2.34048600	-2.06728700
N	-1.12125100	1.94443400	-0.47435600
C	-2.44444400	1.73126800	-0.37838800
N	-2.88213500	0.53984600	0.06605200
C	-4.22913500	0.21190700	0.41556800
C	-4.90668200	0.89094500	1.43113200
C	-4.83327000	-0.86172900	-0.23400000
C	-6.20409900	0.51260900	1.76548800
C	-6.13383400	-1.23583000	0.11521400
H	-4.28971100	-1.40266200	-1.00089500
C	-6.82782200	-0.55148400	1.10849700
H	-7.83444500	-0.84695500	1.37767400
C	-6.76721600	-2.39255400	-0.61412700
C	-6.96205600	1.28604100	2.81218300
F	-6.08325100	-3.54067700	-0.41956900
F	-8.04049500	-2.60700100	-0.22457500
F	-6.78564300	-2.17651200	-1.95287800
F	-7.71029000	2.26807300	2.25891300
F	-7.80552500	0.49326700	3.50640400
F	-6.13148500	1.87752100	3.69992600
S	-3.56669400	3.02539100	-0.71494200
H	-4.42311900	1.70128300	1.96120800
H	-2.25245000	-0.27411600	0.12159400
H	-0.45737600	1.23942000	-0.10354200
C	-2.06772600	4.48143100	1.50557800
H	-1.98831300	5.47393100	1.06766400
H	-2.73856400	3.88057500	0.44984400
H	-2.83351000	4.38668400	2.27610200
C	-0.26760100	5.42589600	-1.17972600
H	0.28563800	6.25284700	-0.71762600
H	-1.28268500	5.47828700	-0.78264600
C	1.87369800	4.00760100	-1.04314000
C	2.68732800	5.11836200	-0.75071300
C	2.51282300	2.85567200	-1.52151100
C	4.06530700	5.09497900	-0.95977000
H	2.24980600	6.02747900	-0.34941800
C	3.89402400	2.82889400	-1.73358700
H	1.96313000	1.94308300	-1.70649500
C	4.67888900	3.94673900	-1.46187100
H	4.65725900	5.97665200	-0.72762000
H	4.35005300	1.91266500	-2.09775600
H	5.75271500	3.92251000	-1.62634400
C	-0.37213300	5.67662000	-2.67785700
C	-1.57859800	5.77652900	-3.25123800

H	-1.68814000	5.99090000	-4.31162700
H	-2.49911100	5.64808600	-2.68739300
C	-0.87861800	2.61064200	2.66210300
H	-1.86601300	2.37700900	3.07114300
H	-0.39458400	1.70115100	2.29346800
H	-0.24800000	2.96347300	3.49385500
C	0.88523200	5.86597800	-3.49322300
H	1.47426000	4.94426500	-3.55420100
H	0.63996900	6.18203600	-4.51217700
H	1.54261500	6.62310200	-3.04799100

TS-EF-5R

l imaginary frequency

H = -5315.354609

G = -5315.555626

E(M06-2X-DCM) = -5316.242730

O	-0.86571900	-2.42447000	-0.68797700
O	-2.81411200	-0.83165800	-0.04573800
P	-1.17826500	-0.93567400	-0.07486000
O	-0.68757900	0.16938800	-0.95606100
C	-2.02884800	-3.03874400	-4.66132200
C	-2.93481000	-3.20748800	-3.61921200
C	-2.51635800	-3.08212700	-2.28703700
C	-0.26025800	-2.53459800	-3.04147700
C	-0.69960200	-2.73985900	-4.36154100
C	-3.56825300	-1.77351600	0.65503500
C	-3.82317000	-3.01976600	0.07967700
C	-4.44805500	-4.01258200	0.85228500
C	-4.90986300	-3.73508800	2.13386200
C	-4.75663500	-2.44609500	2.64199500
C	-4.08190300	-1.44397400	1.92595500
H	0.02414700	-2.63931700	-5.16499800
H	-5.14995000	-2.20059100	3.62413800
C	-3.62758000	-3.53227800	-1.34685100
C	-4.87947800	-3.22697400	-2.23775800
H	-5.12810800	-2.16365600	-2.13979900
H	-5.75896700	-3.80496600	-1.93704100
H	-5.52601900	-5.52974700	-0.26038300
H	-4.21110900	-6.17624600	0.71537900
C	-1.21221600	-2.67828200	-2.01361800
H	-2.34323200	-3.14640000	-5.69651300
H	-5.39551100	-4.50400800	2.72934400
C	-4.41424400	-3.52125200	-3.68161100
H	-4.94172800	-2.91514100	-4.42727500

H	-4.58862500	-4.57229000	-3.95161100
C	-4.50733600	-5.32172200	0.09634100
C	-3.53868000	-5.07257200	-1.07816400
H	-2.51504600	-5.31546500	-0.77103000
H	-3.77003400	-5.66558500	-1.96846000
C	-4.00949100	-0.06987900	2.51736800
C	-3.25293800	0.16481000	3.69059800
C	-4.80403200	0.96641700	1.96504600
C	-2.41549000	-0.83466500	4.28103500
C	-3.30182300	1.46277300	4.32725300
C	-4.81866200	2.26929300	2.59226000
C	-1.70094100	-0.58152900	5.42152000
H	-2.32020600	-1.79266000	3.78759200
C	-2.55250300	1.68021900	5.52671100
C	-4.07383100	2.47992700	3.75709800
C	-1.77758600	0.68761100	6.06236500
H	-1.04930600	-1.34925300	5.82739700
H	-2.61159000	2.65740500	6.00097900
H	-4.11058800	3.45434000	4.24139700
H	-1.20723800	0.86661800	6.96983600
C	1.18128200	-2.21971200	-2.79237600
C	1.74907600	-1.03708200	-3.32965500
C	2.00209400	-3.15096400	-2.10734700
C	0.97252100	-0.03314400	-3.99640000
C	3.17156700	-0.80579800	-3.20696700
C	3.41361100	-2.88091500	-1.95112400
C	1.56214400	1.07490500	-4.55031800
H	-0.10319500	-0.15199300	-4.04803100
C	3.74729600	0.36140100	-3.80365100
C	3.96222800	-1.72486400	-2.51236600
C	2.97044900	1.27440500	-4.46555500
H	0.94621100	1.81007100	-5.06229100
H	4.82353800	0.49875800	-3.72306200
H	5.02808900	-1.53305600	-2.40581900
H	3.42105100	2.15153300	-4.92245300
C	-6.40781500	1.79649800	0.31320800
H	-7.04226400	1.61933800	-0.55124600
C	-5.64243200	0.77682900	0.81852900
H	-5.67803500	-0.20255000	0.35499700
C	-6.39090700	3.08670700	0.91574400
H	-7.00049700	3.88410800	0.49955600
C	-5.62021100	3.30989800	2.02481300
H	-5.61251600	4.28482300	2.50717300
C	2.32317800	-5.25612300	-0.90762400

H	1.91406200	-6.18035500	-0.50846400
C	3.70649000	-4.97020700	-0.73264300
H	4.33882600	-5.67283200	-0.19683200
C	4.23295500	-3.81694800	-1.24653000
H	5.28987000	-3.58887700	-1.13146000
C	1.50457800	-4.38238300	-1.57352900
H	0.45675200	-4.62561200	-1.70326100
C	-1.18273700	3.84405500	-1.45837600
C	-1.45536400	3.52019800	0.03938300
H	-2.38201100	4.03463900	0.34199400
H	-1.66144300	2.45177000	0.12700400
C	-0.43711300	3.84571500	1.10119700
C	0.31263200	3.51253200	-1.79734300
H	0.93695700	4.39581000	-1.67164100
H	0.39646600	3.20402300	-2.84254700
N	0.89449200	2.44498000	-0.98107900
C	2.13526600	2.45897800	-0.46762400
N	2.65119600	1.29602400	-0.03715900
C	3.98002800	1.11826900	0.45738800
C	5.05292500	1.25298400	-0.42083400
C	4.18913000	0.71685600	1.77829800
C	6.34837100	0.98847200	0.02281300
C	5.49256900	0.46790600	2.21201900
H	3.34429800	0.59084100	2.44754700
C	6.57635000	0.59971000	1.34129800
H	7.58267500	0.39583600	1.68587600
C	5.72613000	-0.00938000	3.62335900
C	7.47617800	1.10878000	-0.96548800
F	5.61292400	-1.35176100	3.71918400
F	4.84005900	0.52880800	4.48526900
F	6.96647500	0.31392000	4.05754400
F	7.21508500	0.38870700	-2.08958700
F	8.64684100	0.66500800	-0.46772800
F	7.66155100	2.38549800	-1.36545000
S	2.99712900	3.95589800	-0.22761300
H	4.86662400	1.53424000	-1.45105700
H	2.08447000	0.43656200	-0.03702700
H	0.40148500	1.53354800	-1.02714600
C	0.42158800	4.94774600	1.10716900
H	0.20352000	5.79620500	0.46388200
H	1.53607900	4.52253300	0.52065100
H	0.85389400	5.21844800	2.07153700
N	-0.72962900	-1.00509600	1.47777800
S	0.77625800	-1.19003600	1.93151300

O	1. 11207200	-0. 32028200	3. 07035600
O	1. 75610500	-1. 22969000	0. 81249700
C	0. 82368000	-2. 92451600	2. 62780100
F	0. 47381000	-3. 81382000	1. 69587100
F	-0. 02135300	-3. 03261000	3. 66569900
F	2. 05992900	-3. 19824700	3. 05448000
C	-2. 12893500	3. 02552900	-2. 37406100
C	-3. 20774900	2. 26902100	-1. 89978000
C	-1. 94391800	3. 07984400	-3. 76805100
C	-4. 05490000	1. 58713400	-2. 77743800
H	-3. 41671400	2. 18785600	-0. 84088900
C	-2. 78459600	2. 39983000	-4. 64673800
H	-1. 13667200	3. 67318400	-4. 18974600
C	-3. 84952600	1. 64461900	-4. 15323500
H	-4. 87582400	1. 00752000	-2. 36603200
H	-2. 60810300	2. 46572400	-5. 71723000
H	-4. 50765300	1. 11096600	-4. 83346600
C	-1. 38993300	5. 37331500	-1. 78850300
H	-0. 61957200	5. 94884800	-1. 26838900
H	-1. 18602000	5. 50575600	-2. 85846300
C	-2. 74261800	5. 98654900	-1. 46247100
C	-2. 91301400	6. 69090900	-0. 33584400
H	-2. 10938000	6. 83960500	0. 38186500
H	-3. 86470200	7. 15687100	-0. 09310600
C	-0. 40423700	2. 89932300	2. 25722300
H	0. 34922300	3. 16741800	3. 00122900
H	-1. 39063700	2. 90047900	2. 74514500
H	-0. 24508100	1. 86138200	1. 94374900
C	-3. 86279200	5. 83964600	-2. 46521000
H	-4. 74044300	6. 41770700	-2. 15954600
H	-3. 54670000	6. 19683000	-3. 45440700
H	-4. 16577000	4. 79563100	-2. 59185000

TS-EF-5R-1

l imaginary frequency

H = -5315. 353700

G = -5315. 554631

E(M06-2X-DCM) = -5316. 242832

O	-1. 06123400	-2. 09344200	-1. 36154800
O	-2. 83365000	-0. 58140700	-0. 20817200
P	-1. 22147800	-0. 84860900	-0. 30345700
O	-0. 59872000	0. 41208500	-0. 81749100
C	-2. 17329700	-1. 27277900	-5. 31398500
C	-3. 12468400	-1. 63570300	-4. 36564300

C	-2.73266600	-1.99626500	-3.06838300
C	-0.40297400	-1.53688400	-3.63815900
C	-0.82561800	-1.26425000	-4.95182300
C	-3.70322400	-1.60805800	0.16031500
C	-4.09293500	-2.55058700	-0.79383800
C	-4.85370100	-3.65922000	-0.38820100
C	-5.30687800	-3.77354900	0.92091600
C	-5.00363300	-2.76195800	1.82979100
C	-4.19525600	-1.66718000	1.48023800
H	-0.07121400	-1.01758200	-5.69310900
H	-5.38183300	-2.81687500	2.84632500
C	-3.92107300	-2.57918700	-2.31248500
C	-5.09471400	-1.83631200	-3.03567400
H	-5.20089100	-0.83781600	-2.59582800
H	-6.05148900	-2.35609700	-2.92454700
H	-6.08450500	-4.56317000	-1.92704700
H	-4.89070500	-5.66386700	-1.24662000
C	-1.39636000	-1.87208800	-2.69575400
H	-2.46716300	-1.01238100	-6.32795000
H	-5.89808500	-4.63078500	1.23287000
C	-4.63024700	-1.71103000	-4.50421000
H	-5.05034100	-0.83202100	-5.00684600
H	-4.93364400	-2.58536600	-5.09691600
C	-5.05809900	-4.62061100	-1.53775800
C	-4.03337500	-4.11951300	-2.57525400
H	-3.05729000	-4.57893800	-2.38190900
H	-4.31069500	-4.34770300	-3.60903600
C	-3.96766100	-0.60779400	2.51564000
C	-3.22893300	-0.90799400	3.68616600
C	-4.61968000	0.64514600	2.38916800
C	-2.52297900	-2.14138700	3.85823000
C	-3.16099900	0.05914000	4.75955100
C	-4.52226100	1.61376200	3.45918600
C	-1.82527100	-2.40813100	5.00611000
H	-2.51152500	-2.85339400	3.04372900
C	-2.43469300	-0.26591600	5.94831600
C	-3.80423100	1.29232900	4.61556000
C	-1.78886900	-1.46571300	6.07253700
H	-1.27243700	-3.33839300	5.09375200
H	-2.40464800	0.46815600	6.75046200
H	-3.75946400	2.01321800	5.43031700
H	-1.23356700	-1.69872200	6.97704300
C	1.05691200	-1.48470200	-3.31319500
C	1.77374800	-0.27212500	-3.47611500

C	1. 74354000	-2. 66404800	-2. 92819100
C	1. 14732100	0. 96267700	-3. 84724700
C	3. 20347700	-0. 24927500	-3. 26167400
C	3. 16553200	-2. 61378500	-2. 67341600
C	1. 87406500	2. 11051700	-4. 03708600
H	0. 07221000	0. 97767700	-3. 97824900
C	3. 92804000	0. 96650200	-3. 47956800
C	3. 85757300	-1. 41300300	-2. 85059000
C	3. 28801200	2. 11525200	-3. 86148300
H	1. 36853700	3. 02669700	-4. 33274800
H	5. 00598500	0. 95048600	-3. 33655500
H	4. 92943700	-1. 38082700	-2. 66611200
H	3. 85076000	3. 02910700	-4. 03197800
C	-6. 06043300	2. 20364600	1. 17346100
H	-6. 66793900	2. 43380500	0. 30273900
C	-5. 42205200	0. 99358000	1. 25533000
H	-5. 52959900	0. 27563800	0. 45067600
C	-5. 94109500	3. 16258300	2. 21931300
H	-6. 45839200	4. 11538900	2. 14022900
C	-5. 19236800	2. 87110600	3. 32825400
H	-5. 10837500	3. 58531300	4. 14467300
C	1. 78852700	-5. 05490900	-2. 42341600
H	1. 26843100	-6. 00487600	-2. 33426000
C	3. 18239300	-4. 99142500	-2. 14288300
H	3. 71198400	-5. 88892800	-1. 83527900
C	3. 84833900	-3. 80327700	-2. 27040100
H	4. 91541900	-3. 73985800	-2. 07149000
C	1. 09727500	-3. 93493800	-2. 80413400
H	0. 03822500	-4. 00870700	-3. 02120500
C	-1. 12902000	4. 24075400	-0. 15321800
C	-1. 46381900	3. 50201700	1. 19805900
H	-2. 30672700	4. 02613000	1. 67473100
H	-1. 84513100	2. 50864200	0. 94785600
C	-0. 40751800	3. 32955400	2. 26382900
C	0. 34201600	3. 95330400	-0. 56679700
H	0. 99413200	4. 71032900	-0. 13785700
H	0. 45164200	4. 04741700	-1. 65135400
N	0. 85913200	2. 64583500	-0. 15212300
C	2. 09508300	2. 42852400	0. 32838200
N	2. 55022500	1. 16498500	0. 35570000
C	3. 86431100	0. 77583100	0. 76893300
C	4. 03830500	-0. 01642300	1. 90520800
C	4. 95194400	1. 11477700	-0. 03241600
C	5. 32168400	-0. 45598300	2. 23445800

C	6. 22638400	0. 65530900	0. 30046600
H	4. 79313900	1. 70487500	-0. 92781400
C	6. 41929300	-0. 12880800	1. 43584100
H	7. 40732700	-0. 49354800	1. 68826000
C	7. 35945300	0. 95858500	-0. 64078800
C	5. 52914800	-1. 25777000	3. 49467600
F	7. 19482900	0. 31095900	-1. 82727800
F	8. 55566100	0. 58404800	-0. 14793000
F	7. 42826300	2. 27507300	-0. 93409800
F	5. 70222400	-0. 44905400	4. 56722000
F	6. 62975700	-2. 03989200	3. 41245400
F	4. 47845000	-2. 05346500	3. 76297000
S	3. 02757700	3. 72059200	1. 03775300
H	3. 18066100	-0. 30619600	2. 50310200
H	1. 94751600	0. 38514200	0. 06401600
H	0. 32814500	1. 81118600	-0. 46444600
C	0. 50202000	4. 30891600	2. 66328300
H	0. 32229800	5. 34769900	2. 39628000
H	1. 60673700	4. 07776600	1. 93282800
H	0. 96436000	4. 17143200	3. 64191500
N	-0. 80563300	-1. 44120000	1. 14004400
S	0. 68688300	-1. 82779800	1. 51445800
O	1. 03464600	-1. 38724900	2. 87423600
O	1. 67848900	-1. 54636600	0. 44378100
C	0. 64431400	-3. 69418800	1. 61468000
F	-0. 20885700	-4. 09216800	2. 57175800
F	1. 86406000	-4. 15089800	1. 91392400
F	0. 25367200	-4. 21657200	0. 44983200
C	-2. 16987800	3. 74494600	-1. 18337900
C	-1. 83300100	2. 96083800	-2. 29461000
C	-3. 52744000	4. 06153700	-1. 00280600
C	-2. 80356000	2. 54020700	-3. 20716600
H	-0. 81176800	2. 64128300	-2. 45953400
C	-4. 49830300	3. 64945200	-1. 91356900
H	-3. 84578200	4. 63302500	-0. 13569200
C	-4. 13959900	2. 89174400	-3. 02883200
H	-2. 50856700	1. 92411200	-4. 05231200
H	-5. 53713100	3. 92202500	-1. 74788900
H	-4. 89395200	2. 57176600	-3. 74263600
C	-1. 26143200	5. 79842400	0. 02346800
H	-2. 31294000	6. 02781700	0. 23274200
H	-0. 70412200	6. 08915000	0. 91801400
C	-0. 40379400	2. 00847700	2. 96100900
H	-0. 41349700	1. 16474200	2. 26368700

H	0.43425800	1.89681800	3.65321500
H	-1.33733500	1.91522500	3.53779500
C	-0.78217600	6.67408700	-1.12328000
C	0.33050200	7.40716000	-0.99105700
H	0.93123300	7.38876500	-0.08460400
H	0.68137200	8.06030800	-1.78617800
C	-1.61686700	6.74393300	-2.38057000
H	-1.65574800	5.78191000	-2.90289400
H	-2.65669500	7.00779800	-2.14760300
H	-1.21993300	7.49394900	-3.07166100

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l imaginary frequency

H = -5315.360379

G = -5315.559737

E(M06-2X-DCM) = -5316.242879

O	1.62838700	-2.66539500	-0.30217500
O	2.77870600	-0.36819300	-0.59393600
P	1.31407100	-1.05666900	-0.37036600
O	0.74063200	-0.51678600	0.89911200
C	4.30642500	-4.01476600	2.62713600
C	4.76710400	-3.55999300	1.39644700
C	3.86751400	-3.16223900	0.39560700
C	2.00275500	-3.62110800	1.90194800
C	2.93262000	-4.06299900	2.85835400
C	3.48866900	-0.61320700	-1.77025400
C	4.18682000	-1.80989600	-1.91819700
C	4.71816500	-2.13949300	-3.17477500
C	4.67607800	-1.22610300	-4.22283800
C	4.10972000	0.03036600	-4.00369500
C	3.49356200	0.36312500	-2.78578400
H	2.55636300	-4.43197000	3.80806300
H	4.12027900	0.77337800	-4.79569800
C	4.62053900	-2.85492100	-0.89409600
C	6.02699300	-2.48087500	-0.30757700
H	6.00676700	-1.43151100	0.00855600
H	6.82907600	-2.59138800	-1.04368900
H	6.38405800	-3.53251100	-3.18359800
H	4.95891100	-4.13471600	-4.02202800
C	2.50147500	-3.14696100	0.67358500
H	5.00257400	-4.32740800	3.40135300
H	5.09490700	-1.47383900	-5.19504300
C	6.19459200	-3.38855100	0.92794500
H	6.84007000	-2.94590400	1.69508300

H	6. 64295200	-4. 35506600	0. 65707800
C	5. 28540600	-3. 54379100	-3. 15846700
C	4. 75724700	-4. 10821400	-1. 81927500
H	3. 76408900	-4. 54770800	-1. 96633300
H	5. 40435500	-4. 87846200	-1. 38751800
C	2. 93977300	1. 73906500	-2. 58805700
C	1. 87611500	2. 20777300	-3. 39834400
C	3. 55539900	2. 61014400	-1. 65175900
C	1. 19602800	1. 37472100	-4. 34459600
C	1. 43299900	3. 57918800	-3. 27474500
C	3. 07920900	3. 96847200	-1. 51840500
C	0. 19781700	1. 86836200	-5. 14287000
H	1. 46334100	0. 32705700	-4. 40356600
C	0. 38905200	4. 05599900	-4. 12915100
C	2. 03381800	4. 41569400	-2. 33094800
C	-0. 20383500	3. 23133700	-5. 04791700
H	-0. 30713200	1. 20781400	-5. 84171500
H	0. 08745800	5. 09745600	-4. 03838900
H	1. 68398100	5. 44046800	-2. 22653600
H	-0. 98479300	3. 61023500	-5. 70298200
C	0. 54454900	-3. 70669100	2. 22641700
C	0. 00133100	-2. 88792500	3. 24568100
C	-0. 26183600	-4. 68027400	1. 58821900
C	0. 75821400	-1. 86799000	3. 90952300
C	-1. 37616600	-3. 06508100	3. 64534500
C	-1. 64188700	-4. 83688800	1. 98748000
C	0. 20825600	-1. 10423800	4. 90659200
H	1. 78162800	-1. 69097000	3. 60089900
C	-1. 91089300	-2. 24889700	4. 69184900
C	-2. 15767600	-4. 03229400	3. 00780800
C	-1. 14402700	-1. 29928900	5. 31046800
H	0. 80663200	-0. 33360500	5. 38403400
H	-2. 94707500	-2. 40319100	4. 98482600
H	-3. 19171100	-4. 16808000	3. 31906300
H	-1. 56228800	-0. 68664000	6. 10472100
C	5. 23117400	3. 08408300	0. 06703500
H	6. 06495400	2. 75371100	0. 68032500
C	4. 66295800	2. 21964100	-0. 83158100
H	5. 06090200	1. 21680500	-0. 93038300
C	4. 74309900	4. 41372200	0. 20590400
H	5. 20628500	5. 08630800	0. 92296400
C	3. 69950000	4. 84076900	-0. 56951700
H	3. 31744500	5. 85337300	-0. 47526700
C	-0. 56682400	-6. 49421200	-0. 02132300

H	-0.16146400	-7.14225200	-0.79380400
C	-1.92972200	-6.63376700	0.36574500
H	-2.55260400	-7.38287500	-0.11568900
C	-2.44654200	-5.82917800	1.34457700
H	-3.48374300	-5.93051800	1.65532400
C	0.23680600	-5.55556100	0.57070200
H	1.27415300	-5.46928500	0.26846700
N	0.52972000	-0.86357800	-1.77876900
S	-0.98602100	-1.17471400	-2.03008400
O	-1.58489900	-0.24520600	-3.00711300
O	-1.79868100	-1.42335700	-0.80108400
C	-1.01708300	-2.82506300	-2.90593500
F	-0.33296300	-2.74635200	-4.05235000
F	-2.28772500	-3.15123200	-3.18281700
F	-0.48051900	-3.77506400	-2.14002500
C	-5.23705200	0.23712400	-0.60709700
C	-4.51968000	0.97140300	-1.78283000
H	-5.19040400	0.98609000	-2.65613800
H	-3.66087200	0.37944100	-2.11239500
C	-4.06918500	2.38729800	-1.61824400
C	-4.44127800	0.46258400	0.72190000
H	-4.85373900	1.29787400	1.28124600
H	-4.54178900	-0.43205300	1.34617200
N	-3.01414000	0.75613900	0.55595200
C	-2.34472700	1.71772600	1.23548700
N	-1.00560700	1.58032500	1.30407400
C	-0.06326000	2.52165700	1.80431900
C	-0.06308300	3.86206800	1.41602100
C	0.94534300	2.03835700	2.64580800
C	0.91644100	4.72419600	1.91095700
C	1.92534600	2.90794200	3.11778800
H	0.96076400	0.98813700	2.90831300
C	1.91112400	4.25883200	2.76753500
H	2.67307900	4.93184500	3.14114400
C	3.05503800	2.38856200	3.96723500
C	0.86907100	6.17554400	1.51637600
F	2.75735000	1.20374700	4.54846900
F	4.18011900	2.20228300	3.24246300
F	3.36877400	3.25643500	4.95699600
F	2.05520200	6.79574100	1.70642800
F	0.54323700	6.32628600	0.20812200
F	-0.05480100	6.86243700	2.22467700
S	-3.17316600	3.07168300	1.93136200
H	-0.81091200	4.23186500	0.72775000

H	-0.56753600	0.66828500	1.06870700
H	-2.45280000	0.00119100	0.13251300
C	-4.70062800	3.31458800	-0.76623700
H	-5.72103400	3.09094600	-0.45557500
H	-4.08689100	3.21390700	0.31211000
H	-4.51953300	4.36721100	-0.99468500
C	-5.20388400	-1.29074200	-1.01954700
H	-4.15410800	-1.56474300	-1.15936500
H	-5.68601400	-1.36656900	-2.00354500
C	-6.70741400	0.68162700	-0.44024000
C	-7.30281200	0.86297400	0.81954700
C	-7.53600500	0.83925400	-1.56581000
C	-8.65074500	1.20829000	0.94695000
H	-6.72964500	0.71725200	1.72806500
C	-8.88091700	1.18559500	-1.44409000
H	-7.14097300	0.67546700	-2.56447100
C	-9.44751300	1.37754500	-0.18341700
H	-9.07395200	1.34017200	1.93908900
H	-9.48629800	1.30148100	-2.33917000
H	-10.49481900	1.64874500	-0.08516400
C	-5.84209100	-2.29448800	-0.07530700
C	-5.08550600	-2.96265500	0.80556900
H	-4.01015000	-2.81940800	0.87165600
H	-5.51814800	-3.70481800	1.47310600
C	-2.89683000	2.80935200	-2.43545500
H	-2.51017400	3.78847200	-2.14191300
H	-2.10178300	2.05618200	-2.43605200
H	-3.21938300	2.88144900	-3.48667400
C	-7.31745900	-2.58768000	-0.22235600
H	-7.94151300	-1.70610200	-0.04457700
H	-7.53903700	-2.92881600	-1.24324300
H	-7.63332600	-3.37457700	0.46995600

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l imaginary frequency

H = -5315.351510

G = -5315.552329

E(M06-2X-DCM) = -5316.236460

O	-2.30422400	-1.52133800	-0.95211100
O	-1.67414000	-1.64951300	1.56908500
P	-1.24226900	-0.95112700	0.15197400
O	-1.32677200	0.53162700	0.36533900
C	-6.46187700	-1.41020400	-0.43356500
C	-5.69302000	-2.38058200	0.19833100

C	-4.30838300	-2.45804900	-0.02105200
C	-4.44217500	-0.50222700	-1.48032300
C	-5.83592800	-0.50615800	-1.28740300
C	-1.46698100	-3.02135000	1.73701500
C	-2.35467400	-3.92531700	1.15895300
C	-2.02351000	-5.28964600	1.13542900
C	-0.89948900	-5.75693700	1.80653200
C	-0.10663400	-4.84981200	2.50925700
C	-0.35556400	-3.46750300	2.47776400
H	-6.42929600	0.23221700	-1.81794400
H	0.74863300	-5.20547900	3.07595300
C	-3.76332700	-3.74048100	0.60406700
C	-4.81557400	-3.95780500	1.74631800
H	-4.53546900	-3.33366800	2.60288700
H	-4.85079000	-4.99598100	2.08916000
H	-3.67802200	-6.68468100	0.94047700
H	-2.54022900	-6.74477100	-0.40131500
C	-3.68631800	-1.47880800	-0.79796700
H	-7.53666600	-1.36215700	-0.27790300
H	-0.64412800	-6.81352700	1.79815900
C	-6.14809500	-3.45931600	1.15447600
H	-6.83769400	-3.08066200	1.91767600
H	-6.67703200	-4.26275400	0.62271200
C	-3.02638700	-6.06557400	0.30826700
C	-3.82008500	-4.94238200	-0.39648000
H	-3.30432400	-4.65283900	-1.31837300
H	-4.84486100	-5.22740600	-0.65462000
C	0.52795900	-2.55415100	3.26721000
C	1.90692400	-2.45934300	2.95584700
C	0.00824000	-1.88328700	4.40427500
C	2.48408500	-3.07759100	1.79889600
C	2.78564100	-1.70369500	3.82147400
C	0.89284000	-1.09964300	5.23745700
C	3.82861500	-2.99833700	1.54679200
H	1.83647000	-3.58875200	1.09832000
C	4.18535600	-1.65827100	3.52837300
C	2.25468200	-1.03857500	4.92910000
C	4.69835500	-2.29753500	2.43131500
H	4.23219700	-3.45791600	0.64964700
H	4.83453200	-1.10460500	4.20325300
H	2.91971000	-0.46828000	5.57497300
H	5.76114500	-2.25214800	2.21399400
C	-3.87341700	0.50137300	-2.43425200
C	-4.08423600	1.88523700	-2.19622000

C	-3.25930500	0.07638600	-3.64046500
C	-4.67571200	2.38894200	-0.99128500
C	-3.70405600	2.85258800	-3.20238800
C	-2.84381500	1.05911400	-4.61695900
C	-4.92796900	3.72633400	-0.81826000
H	-4.92465800	1.69106800	-0.20080800
C	-3.97955700	4.23974500	-2.98167700
C	-3.08814300	2.41465300	-4.37873000
C	-4.58758400	4.66854900	-1.83129400
H	-5.39130900	4.07258200	0.10183800
H	-3.70691300	4.94746900	-3.76163600
H	-2.81078200	3.14464000	-5.13734800
H	-4.81242700	5.72235900	-1.68757300
C	-1.83318300	-1.31476000	5.91182600
H	-2.88086700	-1.40147400	6.18724100
C	-1.36516800	-1.96925700	4.80216200
H	-2.04411700	-2.57466300	4.21321800
C	-0.96088900	-0.52564400	6.71418000
H	-1.34874400	-0.01544400	7.59190900
C	0.36352500	-0.42633800	6.38304100
H	1.04579400	0.16109600	6.99328700
C	-2.45818200	-1.67770600	-5.14048200
H	-2.30416700	-2.73212600	-5.35087800
C	-2.02449200	-0.70417800	-6.08305600
H	-1.54404000	-1.02254700	-7.00398800
C	-2.22026000	0.62526600	-5.82823300
H	-1.90763800	1.38091900	-6.54511500
C	-3.05952600	-1.30180300	-3.96910300
H	-3.38586200	-2.06199700	-3.27170200
N	0.19450300	-1.56749900	-0.25644000
S	0.77839400	-1.87293500	-1.70801100
O	2.22643000	-2.09299700	-1.57495500
O	0.30690700	-0.96793400	-2.77127400
C	0.14587300	-3.57903100	-2.17651500
F	0.32342000	-4.43198000	-1.15805400
F	0.83452400	-4.01973100	-3.23388600
F	-1.15724500	-3.56730200	-2.49631600
C	-0.80735800	3.97863300	1.18176100
C	-1.00808200	3.70137700	-0.34213700
H	-1.82659900	4.32831800	-0.72480000
H	-1.36993100	2.67655400	-0.46006200
C	0.13366100	3.90744200	-1.29015000
C	0.49447500	3.26250500	1.67329700
H	1.32906200	3.95642500	1.71347100

H	0.32938400	2.88600700	2.68837600
N	0.94682900	2.14265800	0.83785700
C	2.21364500	1.96514600	0.42223900
N	2.58141200	0.74164700	-0.01028000
C	3.84364900	0.47212900	-0.64253700
C	3.90450300	0.32993400	-2.02809900
C	4.99092400	0.33549800	0.13565900
C	5.13271000	0.06912000	-2.63584300
C	6.21415100	0.07271000	-0.48313200
H	4.92519600	0.42784000	1.21274700
C	6.29098200	-0.05766600	-1.86929900
H	7.24220600	-0.26069300	-2.34744000
C	7.44704600	-0.13327800	0.35529800
C	5.22320000	-0.01021300	-4.13776500
F	7.60948700	-1.43869000	0.69386700
F	8.56804300	0.23812300	-0.29853700
F	7.39431600	0.56368500	1.50997800
F	5.49867300	1.20330700	-4.67667900
F	6.20869200	-0.84512600	-4.53487600
F	4.07279300	-0.43528300	-4.69231800
S	3.34115700	3.28756000	0.34760700
H	3.00038100	0.39964200	-2.62063900
H	1.92745000	-0.04435100	0.07323000
H	0.26408400	1.37490900	0.71540300
C	1.13921100	4.86105900	-1.10395400
H	0.95496900	5.67131100	-0.40026800
H	2.06029300	4.20456800	-0.46692600
H	1.71825200	5.14015900	-1.98596200
C	-2.07674600	3.33702800	1.87715100
H	-2.11626500	2.29268700	1.55644500
H	-2.95730900	3.83281600	1.44963600
C	-0.76451800	5.48742400	1.51049200
C	0.12218500	6.03573600	2.45249700
C	-1.69224000	6.36528600	0.92083900
C	0.09995600	7.39616300	2.77128600
H	0.83518400	5.40632400	2.97322500
C	-1.71671000	7.72344100	1.23449000
H	-2.42220000	5.99058600	0.20920900
C	-0.81568600	8.25044100	2.16071200
H	0.80311500	7.78183000	3.50466700
H	-2.44564400	8.37021200	0.75304800
H	-0.83166400	9.30878000	2.40540300
C	-2.16131800	3.38108200	3.39257200
C	-1.79823300	2.31348200	4.11685500

H	-1.87333100	2.30502900	5.20146000
H	-1.43817600	1.39771900	3.65460700
C	-2.75341300	4.60665900	4.05045500
H	-2.17130700	5.51253000	3.85301700
H	-3.76573900	4.79605800	3.66663300
H	-2.82458900	4.47620700	5.13509100
C	0.16112900	3.01595800	-2.48797600
H	1.01765800	3.21146200	-3.13798800
H	0.14766500	1.95608300	-2.20302700
H	-0.76274300	3.16211000	-3.06661900

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l imaginary frequency

H = -5315.351856

G = -5315.552273

E(M06-2X-DCM) = -5316.240907

O	2.18070900	-1.90018800	-0.24966900
O	1.82348400	0.27892600	-1.62973000
P	1.17680700	-0.63103500	-0.42180000
O	1.11535100	0.29555100	0.75886600
C	6.26818000	-1.39575100	0.48417200
C	5.75939400	-1.26884400	-0.80420900
C	4.40046600	-1.50517900	-1.06563300
C	4.02897400	-1.93468400	1.31350600
C	5.40851600	-1.76016700	1.51976300
C	1.86750300	-0.22959200	-2.92808700
C	2.85925800	-1.14634800	-3.27118800
C	2.77884400	-1.80728200	-4.50768700
C	1.80533600	-1.45858700	-5.43682500
C	0.91046900	-0.43405900	-5.12767900
C	0.90813500	0.19183100	-3.87066700
H	5.80129200	-1.90330000	2.52204100
H	0.17355000	-0.11990800	-5.86098400
C	4.16176900	-1.53375600	-2.57365100
C	5.33181000	-0.60603100	-3.05149500
H	5.01512800	0.43845600	-2.94767600
H	5.59396700	-0.77104400	-4.10077600
H	4.64623900	-2.58031200	-5.30224700
H	3.44677100	-3.82751100	-4.97840100
C	3.54178100	-1.75931800	0.00264600
H	7.32387100	-1.22973300	0.68380200
H	1.74489600	-1.96502500	-6.39675400
C	6.49035300	-0.89742900	-2.07533700
H	7.15840100	-0.03880600	-1.94141000

H	7.11458400	-1.72899300	-2.43139000
C	3.84598300	-2.87591600	-4.60943300
C	4.36110000	-2.97301300	-3.15634200
H	3.73036500	-3.66731700	-2.59073000
H	5.39748500	-3.31689200	-3.08194400
C	-0.05553600	1.31085100	-3.61870200
C	-1.45055800	1.06324400	-3.58956400
C	0.43094600	2.64034900	-3.52566600
C	-2.00329400	-0.25648600	-3.64874200
C	-2.37362300	2.17209300	-3.47787000
C	-0.50349900	3.73693800	-3.39521300
C	-3.35739000	-0.46346300	-3.62101000
H	-1.33276300	-1.10460700	-3.67819200
C	-3.78084400	1.91298500	-3.46787900
C	-1.87659100	3.47402200	-3.37946000
C	-4.26293900	0.63312700	-3.54248600
H	-3.74232100	-1.47823900	-3.63112800
H	-4.45937300	2.76026600	-3.39745700
H	-2.57557800	4.30432200	-3.29762700
H	-5.33223500	0.44417200	-3.51356400
C	3.15616500	-2.33623600	2.46043500
C	3.03497300	-1.48684000	3.58912900
C	2.52076800	-3.60395700	2.45588800
C	3.65630000	-0.19798700	3.66713200
C	2.25920000	-1.91870800	4.73052300
C	1.71800600	-4.00491000	3.58906400
C	3.56392100	0.57944800	4.79375000
H	4.21748400	0.16097600	2.81310000
C	2.18184300	-1.07641400	5.88450600
C	1.61061800	-3.15539100	4.69268900
C	2.82344200	0.13360500	5.92668500
H	4.06467600	1.54393400	4.82571400
H	1.60754400	-1.42904700	6.73835900
H	1.01913100	-3.47173700	5.54962200
H	2.77269000	0.75319300	6.81845700
C	2.26345900	4.26345000	-3.50618400
H	3.32732000	4.47794000	-3.55974900
C	1.82439500	2.96737200	-3.58941500
H	2.54327000	2.16623000	-3.71640200
C	1.33930500	5.33688100	-3.35767100
H	1.70427500	6.35886800	-3.30021800
C	-0.00449700	5.07585900	-3.30786500
H	-0.72457000	5.88669200	-3.21930600
C	2.02971100	-5.75639200	1.41054500

H	2. 14797000	-6. 44256700	0. 57651800
C	1. 21373800	-6. 13092700	2. 51446000
H	0. 71235900	-7. 09470800	2. 51140500
C	1. 06880800	-5. 27854300	3. 57389000
H	0. 45732500	-5. 55392100	4. 42975700
C	2. 66081400	-4. 54149300	1. 38393100
H	3. 28147300	-4. 28157400	0. 53515900
N	-0. 21878800	-1. 23641300	-0. 96600400
S	-0. 84836700	-2. 69501400	-0. 73119300
O	-2. 24763700	-2. 65345700	-1. 17567000
O	-0. 53724500	-3. 29532100	0. 57273000
C	-0. 03398900	-3. 82054300	-1. 99832900
F	-0. 02783800	-3. 24319200	-3. 21015400
F	-0. 73183200	-4. 95811100	-2. 07052400
F	1. 23048200	-4. 11908400	-1. 66833800
C	0. 62554800	3. 98735500	1. 43391200
C	0. 83464400	2. 98385800	2. 60223900
H	1. 57792100	3. 39233700	3. 30284600
H	1. 29754800	2. 08257000	2. 19335200
C	-0. 34423200	2. 54444700	3. 42388200
C	-0. 63900800	3. 56468400	0. 59919000
H	-1. 50821400	4. 14865600	0. 89541600
H	-0. 45329700	3. 77086500	-0. 46104200
N	-1. 00417000	2. 15132500	0. 72004200
C	-2. 26454000	1. 68322400	0. 82863100
N	-2. 48635300	0. 41763900	0. 42698400
C	-3. 71065000	-0. 30452900	0. 60042000
C	-3. 71057000	-1. 47098200	1. 36575500
C	-4. 87282400	0. 11945200	-0. 04090400
C	-4. 89135000	-2. 20098100	1. 50192100
C	-6. 04735900	-0. 61989200	0. 10205800
H	-4. 85320200	1. 00564800	-0. 66308600
C	-6. 06420000	-1. 77968300	0. 87499100
H	-6. 97662100	-2. 35432800	0. 97996000
C	-7. 27617000	-0. 18618100	-0. 65145000
C	-4. 91936600	-3. 42096000	2. 38613500
F	-7. 22164100	-0. 56379600	-1. 95432800
F	-8. 40338000	-0. 71848900	-0. 13574300
F	-7. 41666600	1. 15742900	-0. 64585300
F	-5. 27307700	-3. 09564600	3. 65502300
F	-5. 82014900	-4. 33017400	1. 95295200
F	-3. 71997100	-4. 02535000	2. 45379300
S	-3. 50891100	2. 63928600	1. 56734300
H	-2. 79358300	-1. 82073800	1. 82689000

H	-1.74040900	-0.07570100	-0.08735400
H	-0.25842300	1.46200500	0.52708200
C	-1.44477500	3.35442100	3.72643800
H	-1.34597400	4.43064500	3.59421500
H	-2.30845000	3.07419900	2.79864200
H	-2.04582800	3.05189400	4.58619100
C	1.87301300	3.88017500	0.47329500
H	1.69139700	4.57109200	-0.35610100
H	1.87236600	2.87080500	0.04475600
C	0.45743800	5.45720300	1.86180900
C	0.00556800	6.39751100	0.91738100
C	0.78354700	5.93619800	3.13825100
C	-0.12878500	7.74725100	1.23881000
H	-0.23362900	6.07870800	-0.09338900
C	0.64871500	7.28799400	3.46626300
H	1.14902100	5.25930200	3.90315300
C	0.19032800	8.20134700	2.51961100
H	-0.48301100	8.44480500	0.48442600
H	0.90842700	7.62211100	4.46730500
H	0.08535300	9.25242200	2.77353000
C	3.24248100	4.17057700	1.06959300
C	3.70055300	5.42128000	1.20113500
H	4.68704800	5.62340400	1.61221500
H	3.11439500	6.28571300	0.90282500
C	4.09560700	2.98114000	1.44266400
H	3.61302000	2.34773700	2.19586700
H	4.26398300	2.33571200	0.57016400
H	5.07044600	3.29355200	1.83123400
C	-0.29427100	1.14067900	3.92873500
H	-1.22275000	0.84073100	4.42179900
H	-0.04736600	0.44335000	3.11957100
H	0.52830500	1.04524700	4.65419100

TS-EF-5R-2

l imaginary frequency

H = -5315.353700

G = -5315.554632

E(M06-2X-DCM) = -5316.242840

O	-1.06136600	-2.09284200	-1.36216300
O	-2.83356700	-0.58116000	-0.20799000
P	-1.22141600	-0.84840400	-0.30357700
O	-0.59867900	0.41247100	-0.81718700
C	-2.17391800	-1.27061300	-5.31413300
C	-3.12520800	-1.63380100	-4.36579500

C	-2.73305000	-1.99489900	-3.06872700
C	-0.40338600	-1.53557200	-3.63866700
C	-0.82618400	-1.26238300	-4.95216600
C	-3.70314400	-1.60789400	0.16025000
C	-4.09307200	-2.55000900	-0.79422200
C	-4.85386600	-3.65874400	-0.38892400
C	-5.30685300	-3.77356700	0.92021700
C	-5.00336700	-2.76238100	1.82946200
C	-4.19495200	-1.66752400	1.48023300
H	-0.07185500	-1.01554300	-5.69347100
H	-5.38140400	-2.81769000	2.84603500
C	-3.92141200	-2.57800800	-2.31290100
C	-5.09508100	-1.83473600	-3.03563600
H	-5.20111000	-0.83640600	-2.59537600
H	-6.05188600	-2.35448200	-2.92458900
H	-6.08495900	-4.56198700	-1.92796000
H	-4.89114100	-5.66304100	-1.24814300
C	-1.39667800	-1.87099600	-2.69624000
H	-2.46790000	-1.00980400	-6.32795900
H	-5.89809000	-4.63087600	1.23191200
C	-4.63079900	-1.70891000	-4.50418400
H	-5.05086400	-0.82964900	-5.00640400
H	-4.93437400	-2.58296900	-5.09720700
C	-5.05850300	-4.61965600	-1.53883900
C	-4.03388500	-4.11822000	-2.57627800
H	-3.05781200	-4.57780800	-2.38325800
H	-4.31137000	-4.34596600	-3.61011200
C	-3.96705100	-0.60862500	2.51606400
C	-3.22823000	-0.90946800	3.68636900
C	-4.61885300	0.64449300	2.39021900
C	-2.52244400	-2.14304700	3.85779600
C	-3.16000500	0.05717700	4.76017500
C	-4.52112100	1.61262500	3.46064600
C	-1.82465300	-2.41041800	5.00547900
H	-2.51117900	-2.85468300	3.04296800
C	-2.43362500	-0.26853100	5.94871600
C	-3.80302700	1.29054700	4.61680100
C	-1.78798800	-1.46849000	6.07232900
H	-1.27195100	-3.34080300	5.09264000
H	-2.40336700	0.46518000	6.75118400
H	-3.75803800	2.01106700	5.43187300
H	-1.23262600	-1.70199700	6.97667100
C	1.05654900	-1.48374400	-3.31387400
C	1.77357200	-0.27123200	-3.47643700

C	1. 74302000	-2. 66334400	-2. 92936500
C	1. 14731700	0. 96380600	-3. 84706500
C	3. 20332200	-0. 24869000	-3. 26211000
C	3. 16503800	-2. 61340100	-2. 67467900
C	1. 87423200	2. 11159400	-4. 03656700
H	0. 07219600	0. 97902700	-3. 97794800
C	3. 92806800	0. 96704500	-3. 47963400
C	3. 85725700	-1. 41266800	-2. 85147800
C	3. 28819500	2. 11603300	-3. 86109100
H	1. 36882500	3. 02796500	-4. 33184400
H	5. 00601800	0. 95080900	-3. 33669600
H	4. 92913400	-1. 38072600	-2. 66704000
H	3. 85107900	3. 02985500	-4. 03131900
C	-6. 05944600	2. 20380200	1. 17535700
H	-6. 66701700	2. 43444800	0. 30480900
C	-5. 42130100	0. 99356900	1. 25663300
H	-5. 52911100	0. 27598400	0. 45169600
C	-5. 93978600	3. 16226900	2. 22160300
H	-6. 45690800	4. 11520900	2. 14299500
C	-5. 19099000	2. 87016100	3. 33033300
H	-5. 10676600	3. 58399600	4. 14705400
C	1. 78767900	-5. 05440500	-2. 42551100
H	1. 26744600	-6. 00433000	-2. 33669400
C	3. 18157000	-4. 99124000	-2. 14503200
H	3. 71104100	-5. 88893800	-1. 83779500
C	3. 84768900	-3. 80314500	-2. 27214500
H	4. 91479000	-3. 73996000	-2. 07327400
C	1. 09657100	-3. 93418500	-2. 80575700
H	0. 03749900	-4. 00771500	-3. 02279900
C	-1. 12926400	4. 24072300	-0. 15226900
C	-1. 46416000	3. 50162600	1. 19880200
H	-2. 30705000	4. 02565700	1. 67559500
H	-1. 84548900	2. 50832900	0. 94833000
C	-0. 40786700	3. 32888600	2. 26453000
C	0. 34193300	3. 95377400	-0. 56555000
H	0. 99378200	4. 71065200	-0. 13595000
H	0. 45191000	4. 04855300	-1. 65001400
N	0. 85906300	2. 64613500	-0. 15142000
C	2. 09497600	2. 42865100	0. 32909600
N	2. 55011300	1. 16510000	0. 35607700
C	3. 86421900	0. 77587400	0. 76920200
C	4. 95187200	1. 11508200	-0. 03202400
C	4. 03819700	-0. 01675900	1. 90520400
C	6. 22629500	0. 65547700	0. 30071400

C	5.32157300	-0.45644700	2.23432900
H	3.18053900	-0.30675800	2.50297500
C	6.41918500	-0.12902900	1.43583600
H	7.40721100	-0.49385600	1.68815100
C	5.52886300	-1.25869400	3.49428300
C	7.35937500	0.95890600	-0.64047900
F	5.69996300	-0.45037700	4.56743800
F	6.63044700	-2.03949800	3.41265100
F	4.47883500	-2.05576400	3.76115300
F	7.19503200	0.31106500	-1.82688700
F	8.55563100	0.58474000	-0.14745100
F	7.42788500	2.27537000	-0.93397200
S	3.02741700	3.72048800	1.03896200
H	4.79309000	1.70548900	-0.92722000
H	1.94748600	0.38535700	0.06396900
H	0.32804400	1.81160800	-0.46401500
C	0.50146500	4.30826200	2.66443600
H	0.32163400	5.34710100	2.39772300
H	1.60638500	4.07736600	1.93415000
H	0.96365000	4.17054100	3.64311000
N	-0.80541800	-1.44155700	1.13964800
S	0.68715300	-1.82831700	1.51371100
O	1.03506900	-1.38835200	2.87363800
O	1.67862100	-1.54641400	0.44303200
C	0.64459700	-3.69475200	1.61313800
F	-0.20828900	-4.09313700	2.57030100
F	1.86442800	-4.15160400	1.91181200
F	0.25359400	-4.21662900	0.44818300
C	-2.16975800	3.74493900	-1.18278800
C	-1.83241800	2.96152700	-2.29436200
C	-3.52746900	4.06090400	-1.00223400
C	-2.80268900	2.54095300	-3.20725200
H	-0.81102100	2.64252000	-2.45933400
C	-4.49804800	3.64888500	-1.91332800
H	-3.84613600	4.63182900	-0.13486700
C	-4.13889300	2.89186200	-3.02891200
H	-2.50735000	1.92539800	-4.05267000
H	-5.53700700	3.92097100	-1.74766200
H	-4.89302400	2.57193200	-3.74297100
C	-1.26212200	5.79832200	0.02474800
H	-2.31372100	6.02736100	0.23394700
H	-0.70498800	6.08899800	0.91942400
C	-0.40392100	2.00754800	2.96120500
H	-0.41393300	1.16407200	2.26358200

H	0.43438700	1.89561400	3.65306100
H	-1.33723400	1.91414700	3.53834100
C	-0.78298900	6.67434700	-1.12177400
C	0.32969800	7.40738900	-0.98945200
H	0.93051600	7.38874400	-0.08306100
H	0.68048300	8.06077000	-1.78441800
C	-1.61780600	6.74453400	-2.37896500
H	-1.65638000	5.78275900	-2.90177100
H	-2.65770700	7.00791000	-2.14578500
H	-1.22118800	7.49503500	-3.06971100

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l imaginary frequency

H = -5315.351926

G = -5315.553090

E(M06-2X-DCM) = -5316.240538

O	-1.32376300	-2.19605900	-1.29282600
O	-2.91791200	-0.53872400	-0.09665100
P	-1.33635700	-0.89916600	-0.28887200
O	-0.70117700	0.30646300	-0.91396600
C	-2.61802600	-1.38653400	-5.19138300
C	-3.53362900	-1.67090700	-4.18295300
C	-3.09153800	-2.03156900	-2.90107600
C	-0.77491000	-1.73706800	-3.61636200
C	-1.25323700	-1.45877800	-4.90854300
C	-3.82438200	-1.49485600	0.36125300
C	-4.34484500	-2.42791300	-0.53732800
C	-5.15541600	-3.46568800	-0.05031700
C	-5.52904700	-3.50938400	1.28812900
C	-5.08704700	-2.50419200	2.14583700
C	-4.22019200	-1.48551400	1.71355400
H	-0.52911700	-1.27152100	-5.69605700
H	-5.39682100	-2.50727900	3.18656000
C	-4.27043800	-2.51076200	-2.06164500
C	-5.43245400	-1.70831600	-2.73872400
H	-5.44992300	-0.69490700	-2.32074400
H	-6.41305100	-2.16014600	-2.55969500
H	-6.54112600	-4.31842400	-1.48406200
H	-5.39035200	-5.48499000	-0.84040000
C	-1.72999700	-1.98977200	-2.61167500
H	-2.95427900	-1.12094200	-6.19058800
H	-6.16246100	-4.30912300	1.66353700
C	-5.04669200	-1.65016500	-4.23402900
H	-5.43869700	-0.75919000	-4.73805000

H	-5.43902900	-2.51800200	-4.78240300
C	-5.49967600	-4.44065700	-1.15433000
C	-4.50670700	-4.04583700	-2.26669100
H	-3.55577200	-4.56949700	-2.11598700
H	-4.86246300	-4.28293000	-3.27415200
C	-3.81545300	-0.43786200	2.70455900
C	-3.06906000	-0.80895600	3.85085900
C	-4.28862700	0.89181700	2.56514300
C	-2.49933900	-2.11247400	4.01446600
C	-2.84166000	0.15685100	4.90246200
C	-4.02786100	1.85597800	3.61164300
C	-1.79177200	-2.44489000	5.13921700
H	-2.59758200	-2.82967300	3.20988100
C	-2.11527100	-0.23745200	6.06981900
C	-3.32986200	1.45877100	4.75658400
C	-1.60861900	-1.50255700	6.19037900
H	-1.34538900	-3.43151800	5.22085800
H	-1.96743500	0.49844000	6.85704700
H	-3.16594100	2.18014100	5.55550900
H	-1.05006900	-1.78804000	7.07766400
C	0.69885800	-1.78052200	-3.36241100
C	1.48620000	-0.61597500	-3.54369900
C	1.31757100	-3.00658200	-3.01051000
C	0.92923400	0.65700300	-3.89686600
C	2.92013400	-0.68701000	-3.36809600
C	2.74742600	-3.05396400	-2.80826600
C	1.72491900	1.75466700	-4.10521100
H	-0.14576800	0.74474700	-3.99904000
C	3.71460800	0.48361300	-3.58753800
C	3.50825100	-1.89728600	-2.99412200
C	3.13950100	1.67099600	-3.95421600
H	1.27359800	2.70122500	-4.39259700
H	4.79183000	0.40551300	-3.45742700
H	4.58631000	-1.94285200	-2.85402500
H	3.75448900	2.54931500	-4.13184800
C	-5.48263800	2.63133100	1.32598400
H	-6.03765700	2.94186000	0.44583900
C	-5.04715100	1.33652300	1.43443400
H	-5.27606300	0.62926100	0.64636800
C	-5.20772700	3.57940100	2.35208300
H	-5.56668300	4.60036900	2.25224400
C	-4.50679600	3.19634600	3.46410300
H	-4.30573600	3.90424200	4.26554000
C	1.22024900	-5.40069700	-2.52772800

H	0.64136800	-6.31490100	-2.42721800
C	2.62517400	-5.43390200	-2.30206700
H	3.10482200	-6.36843500	-2.02423100
C	3.36400900	-4.29126600	-2.44407500
H	4.43965100	-4.30171100	-2.28521400
C	0.59185500	-4.23250100	-2.87079200
H	-0.47746100	-4.23248900	-3.04701500
C	-0.82337500	4.29139700	-0.29273100
C	-1.13606300	3.59453200	1.08360800
H	-1.90990900	4.19464500	1.58528500
H	-1.61476300	2.63707000	0.86172100
C	-0.04290000	3.34132100	2.09393700
C	0.41333700	3.59862200	-0.98697200
H	1.23392300	4.30937600	-1.05606600
H	0.15363400	3.30299800	-2.00505400
N	0.95977600	2.40004500	-0.33797000
C	2.23992900	2.24858200	0.04068400
N	2.71239300	0.99864400	0.17858900
C	4.03554000	0.64565700	0.58283700
C	4.21731500	-0.16481700	1.70520500
C	5.12536100	1.03034300	-0.19812000
C	5.50919500	-0.56975300	2.04788800
C	6.40892500	0.61764200	0.15655300
H	4.96301800	1.61684400	-1.09458700
C	6.60873700	-0.18114900	1.28207200
H	7.60441400	-0.51542300	1.54637000
C	7.57245700	1.05523300	-0.69288800
C	5.71601700	-1.39771700	3.29152700
F	7.26622000	1.00193400	-2.01304400
F	8.66138900	0.28348700	-0.49862800
F	7.93305800	2.33078600	-0.43076300
F	5.77955000	-0.61652600	4.39523300
F	6.87095200	-2.09884700	3.23839600
F	4.71221000	-2.27340300	3.48252700
S	3.20012000	3.63450100	0.49454600
H	3.35980000	-0.48869800	2.28668800
H	2.09445600	0.18855000	0.01570000
H	0.41473600	1.53363100	-0.51550200
C	0.93414000	4.26573900	2.44387500
H	0.78144900	5.31852800	2.22146400
H	1.94123300	4.02373600	1.53373600
H	1.49882700	4.07008600	3.35585000
N	-0.83588400	-1.44033700	1.14697900
S	0.66740900	-1.83672500	1.45575100

O	1.09586300	-1.35850000	2.77868100
O	1.61025400	-1.59773600	0.32778900
C	0.61093100	-3.69885800	1.60882000
F	-0.21040700	-4.05700700	2.60615900
F	1.83689100	-4.15857300	1.87610300
F	0.17382900	-4.24607300	0.47291900
C	-2.12340900	4.11789800	-1.11460600
C	-2.35656300	2.96317200	-1.87905800
C	-3.15669800	5.06558100	-1.03755000
C	-3.55404100	2.78631800	-2.57441000
H	-1.62894400	2.15961500	-1.90920700
C	-4.35359200	4.89180000	-1.73417500
H	-3.03468900	5.96099100	-0.44060900
C	-4.55556100	3.75462500	-2.51598200
H	-3.69753800	1.87907200	-3.15544700
H	-5.12627200	5.65338100	-1.66549800
H	-5.48444800	3.62225700	-3.06471600
C	-0.47695200	5.81048900	-0.08246400
H	-1.11135200	6.21849700	0.71244300
H	0.55036700	5.85652900	0.29844200
C	-0.08639300	2.02029600	2.79346300
H	-0.26543900	1.18149700	2.11593100
H	0.81172400	1.82395100	3.38448000
H	-0.94583100	2.02564700	3.48244400
C	-0.54624300	6.76044400	-1.27132000
C	-1.13108400	7.95615100	-1.13806800
H	-1.62004100	8.26005700	-0.21508400
H	-1.13998900	8.67998900	-1.94885200
C	0.13148100	6.37292400	-2.56297800
H	1.19984600	6.16603500	-2.41451800
H	-0.31662400	5.46998400	-2.99576800
H	0.04628200	7.17388100	-3.30314500

TS-EF-5R-4

l imaginary frequency

H = -5315.348102

G = -5315.548502

E(M06-2X-DCM) = -5316.235903

O	-1.22401500	-2.49632200	-0.84641900
O	-2.91480700	-0.69508700	-0.06237900
P	-1.31445200	-1.01335600	-0.15500900
O	-0.73016400	0.06371000	-1.01972500
C	-2.50795000	-2.67017900	-4.82703200
C	-3.42061900	-2.76662900	-3.78142400

C	-2.97829400	-2.79789300	-2.45037800
C	-0.67074800	-2.54986600	-3.21194400
C	-1.14542100	-2.59957300	-4.53403800
C	-3.78563700	-1.56229500	0.59771600
C	-4.24450500	-2.70362900	-0.06164400
C	-5.01141200	-3.63973300	0.65043400
C	-5.40724900	-3.38806300	1.95932600
C	-5.03122800	-2.18836200	2.56053400
C	-4.20610600	-1.25676100	1.90728300
H	-0.42156000	-2.55710100	-5.34260800
H	-5.36003700	-1.96385200	3.57077300
C	-4.14189700	-3.13465000	-1.52439400
C	-5.33582600	-2.57707600	-2.37113400
H	-5.41670700	-1.49743000	-2.19736800
H	-6.29271300	-3.03069300	-2.09484700
H	-6.32552000	-4.87942000	-0.54983900
H	-5.12613400	-5.79737700	0.35449400
C	-1.62470400	-2.61676200	-2.17774100
H	-2.84447300	-2.65815000	-5.86073600
H	-6.00742900	-4.10966400	2.50777600
C	-4.93148000	-2.84160900	-3.83885100
H	-5.36258000	-2.11252300	-4.53458700
H	-5.26925000	-3.83221700	-4.17412300
C	-5.28492800	-4.86320600	-0.19617200
C	-4.29473800	-4.68557900	-1.36585300
H	-3.32065100	-5.10724600	-1.09283400
H	-4.62087200	-5.16998100	-2.29145300
C	-3.86372100	0.01295500	2.62368700
C	-3.11749400	-0.04074900	3.82744400
C	-4.38694300	1.24950900	2.16679700
C	-2.49855600	-1.24198900	4.30157500
C	-2.93986800	1.15875800	4.61500200
C	-4.17180500	2.44814200	2.94745300
C	-1.79163500	-1.26431800	5.47456700
H	-2.55868600	-2.13555400	3.69382100
C	-2.21273000	1.08715700	5.84475600
C	-3.47292400	2.36708500	4.15607200
C	-1.65839000	-0.08984800	6.26797000
H	-1.30756100	-2.18306100	5.79236600
H	-2.10316300	1.99642400	6.43158300
H	-3.34333500	3.26655400	4.75577600
H	-1.09974600	-0.13005600	7.19911700
C	0.80038600	-2.46199200	-2.95362000
C	1.53233400	-1.32966000	-3.38994100

C	1. 47383200	-3. 54878700	-2. 34103800
C	0. 91596800	-0. 19269900	-4. 00871400
C	2. 96742600	-1. 29344200	-3. 21266800
C	2. 90316900	-3. 48253300	-2. 14015500
C	1. 66005100	0. 86753500	-4. 45994400
H	-0. 16238800	-0. 17645300	-4. 11240100
C	3. 70664900	-0. 16493000	-3. 69193300
C	3. 60991900	-2. 36198800	-2. 58329200
C	3. 07689200	0. 88395000	-4. 30714600
H	1. 16503500	1. 70706800	-4. 94169800
H	4. 78640100	-0. 16366800	-3. 55836600
H	4. 68844600	-2. 32549800	-2. 44387200
H	3. 65026000	1. 72888700	-4. 67937800
C	-5. 63371600	2. 58933400	0. 54235700
H	-6. 19743200	2. 65507800	-0. 38374600
C	-5. 15320300	1. 37686600	0. 96329100
H	-5. 35330800	0. 48974100	0. 37423400
C	-5. 40041200	3. 76877500	1. 30514800
H	-5. 79558500	4. 72047800	0. 95981500
C	-4. 69613200	3. 69378800	2. 47709700
H	-4. 52825000	4. 58241400	3. 08199600
C	1. 48637600	-5. 77712900	-1. 33666700
H	0. 95047400	-6. 67211900	-1. 03205700
C	2. 88998400	-5. 69307100	-1. 11610300
H	3. 41140200	-6. 51849300	-0. 63924300
C	3. 57510900	-4. 57725500	-1. 51261400
H	4. 64907400	-4. 50135100	-1. 36037400
C	0. 80580900	-4. 74572400	-1. 92856200
H	-0. 26128900	-4. 83536200	-2. 09511400
C	-0. 84707400	4. 12328900	-1. 26542100
C	-1. 18185700	3. 67343600	0. 19982100
H	-1. 98030500	4. 31642700	0. 58729600
H	-1. 63047400	2. 67953400	0. 14200000
C	-0. 10624300	3. 62091400	1. 25840900
C	0. 33812000	3. 22431300	-1. 83448200
H	1. 14363400	3. 86726400	-2. 18963100
H	-0. 03075400	2. 64969700	-2. 68565000
N	0. 93645100	2. 23787300	-0. 92705500
C	2. 21607800	2. 21708500	-0. 52313900
N	2. 72324900	1. 04659100	-0. 10112600
C	4. 05121300	0. 83273000	0. 37554500
C	5. 13800900	1. 06987700	-0. 46606800
C	4. 24453400	0. 30278700	1. 65305900
C	6. 42954600	0. 79360100	-0. 02015800

C	5.54439800	0.03105600	2.08533300
H	3.39142500	0.10088300	2.29317800
C	6.64049000	0.27638300	1.25770600
H	7.64445400	0.05919700	1.60149500
C	5.75829900	-0.58722900	3.44441500
C	7.59215900	1.08172800	-0.93255300
F	5.64340800	-1.93211700	3.40049600
F	4.85909900	-0.13836900	4.34278700
F	6.99163800	-0.31108600	3.92696600
F	7.29509400	0.77736500	-2.21975700
F	8.68985400	0.37545500	-0.59179500
F	7.93507600	2.38852300	-0.91167500
S	3.12221300	3.70316300	-0.39206600
H	4.96887500	1.43827200	-1.47079600
H	2.12762200	0.20418900	-0.07238000
H	0.41725100	1.33948000	-0.89888900
C	0.86110800	4.59840300	1.45816000
H	0.71161700	5.59986000	1.06444400
H	1.87831200	4.22906400	0.58321500
H	1.42057600	4.55802700	2.39296900
N	-0.81382100	-1.20296400	1.36803600
S	0.69612500	-1.48075800	1.76236200
O	1.09951900	-0.71705100	2.95246200
O	1.64398400	-1.46479600	0.61311700
C	0.68645100	-3.26552200	2.31808600
F	0.27689300	-4.06082600	1.32810200
F	-0.13752300	-3.41713300	3.36487300
F	1.92036100	-3.62122400	2.68746100
C	-2.11280000	3.85616000	-2.11993300
C	-2.59726000	2.54084700	-2.24738800
C	-2.80143000	4.86996000	-2.80078800
C	-3.72618300	2.25760400	-3.01377300
H	-2.08956200	1.71247600	-1.76130200
C	-3.93514100	4.58590700	-3.56878000
H	-2.46657000	5.89803700	-2.74399000
C	-4.40560400	3.27992000	-3.67896500
H	-4.06654500	1.22829900	-3.09117100
H	-4.44409900	5.39661800	-4.08411300
H	-5.28444500	3.05951200	-4.27942700
C	-0.33582800	5.59520600	-1.41734800
H	0.63757600	5.64204600	-0.91938300
H	-0.09868200	5.72467800	-2.48025300
C	-1.13184100	6.83155000	-0.98973500
C	-0.97423000	7.96356400	-1.68851200

H	-0.35062600	8.01034600	-2.57845100
H	-1.46062200	8.88901500	-1.39121000
C	-0.16354900	2.45372800	2.19258500
H	0.72871100	2.36467000	2.81721200
H	-1.02585000	2.59544300	2.86312900
H	-0.34521800	1.50396100	1.68455800
C	-2.02684400	6.82253300	0.22777900
H	-2.40856700	7.82825400	0.42816400
H	-2.89237000	6.16370700	0.08325000
H	-1.50571300	6.47986700	1.13031100

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l imaginary frequency

H = -5315.352920

G = -5315.553818

E(M06-2X-DCM) = -5316.240214

O	-1.35254000	-2.44747000	-0.82948500
O	-2.99419600	-0.59512600	-0.06048100
P	-1.40295500	-0.95445400	-0.15477300
O	-0.79526500	0.10105800	-1.02958400
C	-2.65067600	-2.64247500	-4.80374000
C	-3.56318500	-2.69858000	-3.75508800
C	-3.11892800	-2.72417500	-2.42460900
C	-0.80704900	-2.55353000	-3.19424500
C	-1.28587300	-2.60776500	-4.51457500
C	-3.88510000	-1.43197300	0.61140200
C	-4.37655200	-2.56742800	-0.03407500
C	-5.16653700	-3.47412900	0.69081400
C	-5.55093800	-3.19721500	1.99807200
C	-5.14033300	-2.00161700	2.58507500
C	-4.29258200	-1.10042500	1.91871100
H	-0.56298300	-2.59857800	-5.32510300
H	-5.45957100	-1.75698800	3.59373800
C	-4.28939500	-3.01734900	-1.49214900
C	-5.46902600	-2.43671500	-2.34328800
H	-5.51876800	-1.35318300	-2.18279800
H	-6.43770800	-2.85969300	-2.05955000
H	-6.51780100	-4.69010000	-0.49246700
H	-5.34181700	-5.63099400	0.41901400
C	-1.76022100	-2.57642800	-2.15736800
H	-2.98926100	-2.63474900	-5.83682200
H	-6.16880100	-3.89612500	2.55621100
C	-5.07572900	-2.73059300	-3.80850600
H	-5.48694400	-1.99751900	-4.51206500

H	-5.44296200	-3.71487300	-4.13122900
C	-5.47619500	-4.69883200	-0.14148500
C	-4.48470100	-4.56163800	-1.31554700
H	-3.52188700	-5.00696500	-1.04006300
H	-4.82654600	-5.04727600	-2.23481600
C	-3.91026500	0.16885100	2.61496400
C	-3.15470800	0.11311600	3.81256000
C	-4.39998100	1.41248200	2.14082700
C	-2.57312700	-1.09906800	4.30563700
C	-2.92805800	1.32136000	4.57370600
C	-4.13441100	2.61857900	2.89366700
C	-1.85651000	-1.12253300	5.47269500
H	-2.67049600	-2.00223600	3.71716300
C	-2.19167200	1.24925800	5.79798000
C	-3.42330500	2.53801900	4.09504900
C	-1.67464400	0.06241100	6.24048600
H	-1.40211900	-2.05118400	5.80525400
H	-2.04488400	2.16587800	6.36491800
H	-3.25472700	3.44469100	4.67379600
H	-1.10884300	0.02151600	7.16728800
C	0.66669600	-2.51051800	-2.93881900
C	1.43524800	-1.40849300	-3.38931500
C	1.30476200	-3.61184500	-2.31427500
C	0.85597600	-0.26006400	-4.02238500
C	2.87095800	-1.41728500	-3.21307900
C	2.73574100	-3.59051400	-2.11531900
C	1.63405700	0.76945100	-4.48722400
H	-0.22141800	-0.21012400	-4.12580100
C	3.64629100	-0.31943700	-3.70622700
C	3.47856900	-2.49897600	-2.57165400
C	3.05073900	0.74153000	-4.33467200
H	1.16630300	1.61897900	-4.97849000
H	4.72579900	-0.35250100	-3.57410300
H	4.55789600	-2.49658800	-2.43349100
H	3.65126500	1.56245500	-4.71768300
C	-5.62835200	2.75977300	0.50893800
H	-6.20783600	2.82531700	-0.40755600
C	-5.18078500	1.54066300	0.94679700
H	-5.42090200	0.64837200	0.38069400
C	-5.34229300	3.94623000	1.24222100
H	-5.70870300	4.90379400	0.88184300
C	-4.62254700	3.87143900	2.40437900
H	-4.41311900	4.76640500	2.98639800
C	1.24510700	-5.82791600	-1.28469500

H	0.68034700	-6.70120400	-0.96943500
C	2.65098500	-5.78771300	-1.06633100
H	3.14551900	-6.62445600	-0.58064000
C	3.37201100	-4.69962200	-1.47598900
H	4.44809900	-4.65749400	-1.32558100
C	0.59817500	-4.78131000	-1.88754400
H	-0.47154700	-4.83741900	-2.05189200
C	-0.64296700	4.13657500	-1.29430400
C	-1.01776000	3.76506200	0.18254400
H	-1.72280200	4.51997400	0.55097400
H	-1.57369900	2.82604700	0.16484800
C	0.06101700	3.64422600	1.23123400
C	0.43492200	3.11470900	-1.86382900
H	1.25480900	3.67000300	-2.32134000
H	-0.02905700	2.50668400	-2.64087900
N	1.01778400	2.14471700	-0.92824200
C	2.29941800	2.08627000	-0.54178600
N	2.77009500	0.90856800	-0.09902200
C	4.08976600	0.65386600	0.37717800
C	5.18562800	0.85510100	-0.46219200
C	4.26304700	0.11723500	1.65514300
C	6.46655900	0.53823900	-0.01262700
C	5.55228500	-0.19646400	2.09036700
H	3.40202500	-0.05547700	2.29342800
C	6.65781100	0.01443400	1.26561200
H	7.65355900	-0.23450700	1.61186400
C	5.74403600	-0.82273400	3.44914900
C	7.64048900	0.78997400	-0.92141200
F	5.60231600	-2.16499600	3.39998800
F	4.84830400	-0.35845700	4.34284300
F	6.97960700	-0.57337000	3.94041500
F	7.33417300	0.50734200	-2.21103400
F	8.71048000	0.04055000	-0.58459400
F	8.03205500	2.08289300	-0.88902400
S	3.25944000	3.54373500	-0.45923900
H	5.03140500	1.22708500	-1.46797700
H	2.14180800	0.08990100	-0.04732700
H	0.46023100	1.27071100	-0.86980900
C	1.06953200	4.57565300	1.41346900
H	0.95311600	5.57603300	1.00616000
H	2.07548300	4.13687000	0.50753800
H	1.64839800	4.51694100	2.33515200
N	-0.90060000	-1.14529900	1.36865800
S	0.59583500	-1.48742400	1.75973200

O	1.04071500	-0.73426500	2.94158900
O	1.53968400	-1.52289800	0.60632600
C	0.51324900	-3.26608000	2.32951600
F	0.06275600	-4.05146000	1.34957000
F	-0.30846900	-3.37353900	3.38344100
F	1.73359100	-3.67135500	2.69323800
C	-1.92209300	3.98174500	-2.16005800
C	-2.56891600	2.73317800	-2.22013800
C	-2.44919300	5.02195700	-2.93838000
C	-3.69993200	2.54247100	-3.01195700
H	-2.18173900	1.88148500	-1.66802900
C	-3.58308200	4.83151000	-3.73348700
H	-1.99474200	6.00515900	-2.92462800
C	-4.21669100	3.59190300	-3.77360400
H	-4.16893800	1.56243300	-3.03492000
H	-3.96519400	5.66146200	-4.32239500
H	-5.09679500	3.44312300	-4.39375600
C	-0.00290400	5.55200600	-1.44371400
H	1.03820500	5.47879100	-1.11338800
H	0.08919200	5.75026400	-2.52282900
C	-0.58571200	6.79999200	-0.79721500
C	-1.83263600	6.95442100	-0.33604100
H	-2.58890100	6.17943200	-0.39216500
H	-2.14906600	7.89998900	0.09770400
C	-0.05224000	2.48395300	2.16932500
H	0.84084800	2.34517800	2.78374300
H	-0.89665600	2.67597700	2.84961400
H	-0.29387000	1.54527300	1.66580500
C	0.39692200	7.95120700	-0.74926400
H	-0.05634900	8.85229800	-0.32616100
H	1.28445900	7.70254700	-0.15079900
H	0.76403600	8.19575900	-1.75552500

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l imaginary frequency

H = -5315.349232

G = -5315.547590

E(M06-2X-DCM) = -5316.229792

O	1.17073300	-2.87482700	-0.33841000
O	2.44737100	-0.67212700	-0.79298300
P	0.93873900	-1.26889200	-0.56005300
O	0.34655100	-0.57671100	0.63030600
C	3.96887000	-4.33079400	2.41655900
C	4.35865300	-3.96195500	1.13363200

C	3. 41566100	-3. 51376400	0. 19613600
C	1. 65399000	-3. 75879600	1. 86825500
C	2. 62191900	-4. 24591600	2. 76340000
C	3. 11602700	-0. 96949600	-1. 98237100
C	3. 67394300	-2. 23203400	-2. 16590200
C	4. 09203500	-2. 61233000	-3. 45016100
C	4. 09602000	-1. 69133300	-4. 49303900
C	3. 71267200	-0. 37320500	-4. 23408800
C	3. 21151600	0. 01788200	-2. 98218500
H	2. 29837200	-4. 55044100	3. 75447500
H	3. 78312800	0. 37538600	-5. 01806600
C	4. 07864500	-3. 30746100	-1. 16208500
C	5. 56138000	-3. 06082600	-0. 70631300
H	5. 66903200	-2. 00719800	-0. 42369800
H	6. 28217300	-3. 26685100	-1. 50326700
H	5. 58441700	-4. 18697100	-3. 57359000
H	4. 03735400	-4. 62521400	-4. 28779100
C	2. 08445500	-3. 36759900	0. 58569800
H	4. 69938100	-4. 68176100	3. 14105100
H	4. 42142000	-1. 97891400	-5. 48971300
C	5. 74860900	-3. 94824100	0. 53977800
H	6. 50098100	-3. 55465400	1. 23270800
H	6. 07179800	-4. 96241600	0. 26460800
C	4. 49735200	-4. 07278000	-3. 46027600
C	4. 01753000	-4. 57368200	-2. 07607800
H	2. 97734100	-4. 91217300	-2. 14167700
H	4. 61680800	-5. 40222400	-1. 68468000
C	2. 90828700	1. 45955800	-2. 70905100
C	1. 82157900	2. 11200200	-3. 33697600
C	3. 78961800	2. 19304400	-1. 87273400
C	0. 89848300	1. 42491200	-4. 18710400
C	1. 60790200	3. 52520400	-3. 11453700
C	3. 55519300	3. 60160600	-1. 64813900
C	-0. 14096000	2. 08437800	-4. 78880900
H	1. 01680200	0. 35843100	-4. 32640200
C	0. 51385200	4. 17598100	-3. 76668700
C	2. 47106200	4. 22760900	-2. 27036100
C	-0. 33371400	3. 48033000	-4. 58561400
H	-0. 83714200	1. 53188300	-5. 41226600
H	0. 37413400	5. 24121500	-3. 59612000
H	2. 29819200	5. 28659400	-2. 09303000
H	-1. 16129200	3. 98630700	-5. 07617100
C	0. 22544600	-3. 72781000	2. 31367700
C	-0. 16325700	-2. 86138000	3. 36375700

C	-0.70372700	-4.64937200	1.77151400
C	0.71554700	-1.87675100	3.92224900
C	-1.49938700	-2.95157800	3.90791500
C	-2.04600700	-4.70721300	2.30411700
C	0.32163800	-1.06800700	4.95741800
H	1.70843300	-1.76340500	3.50385700
C	-1.86677000	-2.10011900	4.99874000
C	-2.40284500	-3.86807000	3.36327700
C	-0.98483500	-1.18709300	5.51379400
H	1.00825400	-0.32482200	5.35076900
H	-2.86675500	-2.20258000	5.41556100
H	-3.40651400	-3.93751100	3.77928300
H	-1.27327700	-0.55503600	6.35015000
C	5.77422600	2.34860900	-0.44967700
H	6.63981800	1.87669900	0.00785600
C	4.93973500	1.61040400	-1.24808300
H	5.15618200	0.56292700	-1.42288600
C	5.52320400	3.72967300	-0.21479600
H	6.19270200	4.29936100	0.42417100
C	4.44503200	4.33507300	-0.80183400
H	4.24283200	5.38915900	-0.63391100
C	-1.28572800	-6.45292700	0.22942000
H	-1.00249800	-7.13428300	-0.56827100
C	-2.61193300	-6.49195500	0.74531400
H	-3.32828800	-7.19924500	0.33604300
C	-2.97607200	-5.64440500	1.75564700
H	-3.98340700	-5.66870400	2.16508400
C	-0.36622000	-5.56734600	0.72625900
H	0.63979700	-5.55603500	0.32386200
C	-5.53896500	1.57561700	0.25912000
C	-5.54147200	1.56398300	1.82666000
H	-5.60468100	2.59966200	2.17768600
H	-6.46914600	1.07784900	2.15694100
C	-4.41499500	0.89324700	2.56057600
C	-4.22693500	2.23185000	-0.27009500
H	-4.25360000	3.28531900	0.00938400
H	-4.21886300	2.18657000	-1.36148900
N	-2.92442300	1.70401100	0.18023300
C	-1.99814600	2.41255300	0.85866700
N	-0.73175800	1.96219600	0.86158700
C	0.37742500	2.59797500	1.49296200
C	0.68616400	3.93546500	1.23334600
C	1.20426900	1.83322300	2.31857600
C	1.79764700	4.51651100	1.84100900

C	2. 32402200	2. 42580400	2. 90497000
H	0. 98147000	0. 78418300	2. 47220200
C	2. 62276400	3. 76843500	2. 68076800
H	3. 49956300	4. 21820500	3. 12951700
C	3. 18662600	1. 61010900	3. 83128800
C	2. 08563200	5. 97534400	1. 60674000
F	2. 65831400	1. 55867700	5. 08364500
F	4. 42721900	2. 12486100	3. 95562400
F	3. 31302500	0. 33284200	3. 41343100
F	1. 76454000	6. 35635200	0. 34663100
F	3. 39066700	6. 27175500	1. 79600400
F	1. 37649200	6. 76615800	2. 44318900
S	-2. 46922400	3. 77387600	1. 85219200
H	0. 07924600	4. 51166000	0. 54648100
H	-0. 51087500	1. 00759200	0. 51626900
H	-2. 54342800	0. 97527300	-0. 44498800
C	-3. 80205500	1. 62930400	3. 57144500
H	-4. 39834900	2. 39463500	4. 07439100
H	-3. 17281800	2. 56422000	2. 83777000
H	-3. 05397100	1. 14206100	4. 19552500
N	0. 16771100	-1. 20205400	-1. 98148900
S	-1. 40632000	-1. 15076900	-2. 04572100
O	-1. 95165700	0. 24186400	-2. 03590700
O	-2. 14768100	-2. 10978400	-1. 20908500
C	-1. 68549300	-1. 73455400	-3. 79609500
F	-1. 01869200	-1. 00304100	-4. 69606000
F	-2. 99954500	-1. 63628600	-4. 06997000
F	-1. 31816200	-3. 00969700	-3. 91939100
C	-5. 87004800	0. 17838100	-0. 29757200
C	-7. 01836100	-0. 49257200	0. 16618200
C	-5. 11097900	-0. 45275900	-1. 28998100
C	-7. 38588500	-1. 73952700	-0. 33276400
H	-7. 65516300	-0. 03695100	0. 92046900
C	-5. 47243200	-1. 70949400	-1. 78792000
H	-4. 21840300	0. 00918300	-1. 69382300
C	-6. 60920300	-2. 35794600	-1. 31471200
H	-8. 28023400	-2. 22681800	0. 04711800
H	-4. 84294400	-2. 17549600	-2. 53707900
H	-6. 88639600	-3. 33487900	-1. 70080300
C	-6. 69290200	2. 58269400	-0. 13456000
H	-6. 50889500	3. 51556800	0. 41190300
H	-7. 63340600	2. 17227600	0. 25457000
C	-3. 99288500	-0. 50878400	2. 26374700
H	-3. 05387900	-0. 76090200	2. 76002200

H	-4.76986100	-1.17990700	2.66346200
H	-3.92140500	-0.73677300	1.19937100
C	-6.87574300	2.92589400	-1.60455300
C	-6.46298900	4.10952900	-2.07530200
H	-5.96852600	4.84279000	-1.44232300
H	-6.60986900	4.39160500	-3.11481300
C	-7.60182400	1.94160300	-2.49127600
H	-7.04830900	1.00442800	-2.60790300
H	-8.57687000	1.67605400	-2.06124300
H	-7.77212000	2.36425400	-3.48619700

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0 imaginary frequency

H = 0.000000

G = -5316.575370

E(M06-2X-DCM) = -5316.245428

O	1.13236500	-2.80345900	0.15573300
O	2.87861300	-0.94668000	-0.25386600
P	1.27544200	-1.18847000	-0.09570100
O	0.80553800	-0.37756900	1.06994900
C	3.07325700	-4.39699900	3.50733600
C	3.74713600	-4.24606700	2.29997000
C	3.08020000	-3.76894000	1.16135500
C	1.03946000	-3.50829100	2.47790900
C	1.72471200	-4.04899300	3.57892600
C	3.56625900	-1.53537900	-1.31676300
C	3.94401200	-2.87402800	-1.23635500
C	4.46400400	-3.50263900	-2.37908700
C	4.72554800	-2.77237000	-3.53362300
C	4.46556200	-1.40100100	-3.54368800
C	3.86686200	-0.75470400	-2.45029200
H	1.18390200	-4.16984100	4.51312300
H	4.70408700	-0.81151500	-4.42409500
C	3.99995000	-3.83949100	-0.05398900
C	5.39590200	-3.75569200	0.65625700
H	5.62522800	-2.70252900	0.85536800
H	6.20338500	-4.16166200	0.03933000
H	5.71297100	-5.24327500	-2.02224600
H	4.26101500	-5.59754700	-2.95155100
C	1.75180700	-3.36208200	1.27225800
H	3.58737400	-4.77349800	4.38810100
H	5.13761000	-3.25583100	-4.41595000
C	5.20506900	-4.50487500	1.99163300
H	5.87337600	-4.14204100	2.78078300

H	5. 40357400	-5. 58026500	1. 87935600
C	4. 65023000	-4. 98476600	-2. 13030700
C	3. 87954400	-5. 20445800	-0. 80862800
H	2. 82184400	-5. 39591900	-1. 02291700
H	4. 25967500	-6. 04420500	-0. 21807800
C	3. 60380400	0. 71712200	-2. 49374300
C	2. 69333600	1. 25473900	-3. 43660900
C	4. 31439000	1. 57869900	-1. 61942400
C	1. 92803700	0. 44062100	-4. 33286100
C	2. 49397600	2. 68566000	-3. 49872400
C	4. 07641200	3. 00306500	-1. 66983100
C	1. 07138500	0. 99596300	-5. 24617400
H	2. 00695200	-0. 63680800	-4. 25790300
C	1. 59243200	3. 22482100	-4. 46979800
C	3. 17542800	3. 51719600	-2. 60643600
C	0. 90739100	2. 40788700	-5. 32787400
H	0. 49276100	0. 35089500	-5. 90121100
H	1. 46858800	4. 30490100	-4. 51031800
H	2. 99593400	4. 58938900	-2. 63536400
H	0. 22932400	2. 82993800	-6. 06546800
C	-0. 39828100	-3. 12238500	2. 63601600
C	-0. 74391600	-2. 04365400	3. 48624500
C	-1. 41145700	-3. 88281300	2. 00353600
C	0. 23532100	-1. 20650500	4. 11399200
C	-2. 13642600	-1. 74153400	3. 72896700
C	-2. 80018800	-3. 56335500	2. 24495900
C	-0. 12830700	-0. 17040900	4. 93477100
H	1. 28328500	-1. 38999200	3. 91114100
C	-2. 47374500	-0. 65861900	4. 60201500
C	-3. 12404700	-2. 51111300	3. 10678100
C	-1. 50270000	0. 10519800	5. 19103200
H	0. 63821000	0. 45705600	5. 38196300
H	-3. 52651100	-0. 45503200	4. 78633600
H	-4. 17210100	-2. 29376100	3. 30795600
H	-1. 77372100	0. 92659100	5. 84888600
C	5. 94489500	1. 96435100	0. 16271200
H	6. 67490000	1. 57486500	0. 86712700
C	5. 28862800	1. 10744900	-0. 68102100
H	5. 51196700	0. 04747400	-0. 64498500
C	5. 68165300	3. 36278800	0. 12909000
H	6. 20684500	4. 02554200	0. 81167700
C	4. 77732700	3. 86420800	-0. 76720400
H	4. 56533600	4. 92888000	-0. 80807100
C	-2. 12851900	-5. 70976300	0. 54740800

H	-1.88160500	-6.54088500	-0.10756000
C	-3.49462500	-5.38449900	0.78127300
H	-4.27661100	-5.96808400	0.30300400
C	-3.81617100	-4.34435200	1.61046200
H	-4.85625700	-4.09285500	1.80658700
C	-1.12588100	-4.98915000	1.14115200
H	-0.09145200	-5.25639000	0.95880600
N	0.64607600	-0.94454300	-1.57042300
S	-0.86772900	-1.12419200	-1.94112500
O	-1.32235000	-0.15209800	-2.95162800
O	-1.78180800	-1.31187000	-0.77503200
C	-0.94295500	-2.76090300	-2.84247700
F	-0.12584100	-2.73262300	-3.90199300
F	-2.19536700	-2.97790000	-3.27409300
F	-0.58428300	-3.76461700	-2.04142000
C	-5.09687400	0.47499400	-0.43830300
C	-4.44744200	1.02391100	-1.73342800
H	-5.13012500	0.84084100	-2.57770900
H	-3.57882100	0.40383200	-1.97599500
C	-4.01079100	2.45432700	-1.83031600
C	-4.19070000	0.80925900	0.81006300
H	-4.56055100	1.69698400	1.32018500
H	-4.24568200	-0.02480900	1.51925500
N	-2.77112400	1.03635400	0.52889200
C	-2.03980400	2.06785800	1.00152500
N	-0.70778100	1.89214700	1.05282900
C	0.27941100	2.86744100	1.36900800
C	0.35062400	4.09910800	0.71284200
C	1.24022300	2.52610600	2.32400200
C	1.35714400	5.00130800	1.05205600
C	2.24746300	3.43572200	2.64635100
H	1.19087500	1.55683200	2.80547700
C	2.30730800	4.68060200	2.02335000
H	3.07739100	5.39304500	2.29401900
C	3.29954700	3.05065400	3.65394700
C	1.45837200	6.31882700	0.33081500
F	2.80733800	2.21403900	4.59746300
F	4.34445900	2.42116500	3.07625700
F	3.79567300	4.13369100	4.29403500
F	1.85449100	7.31046900	1.15708800
F	2.36619500	6.27580000	-0.68042700
F	0.28343300	6.68921500	-0.22065900
S	-2.78661100	3.56274500	1.48043200
H	-0.37541000	4.35552200	-0.04656500

H	-0.31553000	0.92838300	0.99726400
H	-2.25878600	0.21422400	0.17720800
C	-4.50453900	3.48917800	-1.03107500
H	-5.46751900	3.34496400	-0.54404900
H	-3.75884300	3.49090300	0.00927800
H	-4.32091900	4.50576900	-1.38344400
C	-5.15326800	-1.09865700	-0.57816000
H	-5.53112100	-1.48699900	0.37620800
H	-4.12327800	-1.45496000	-0.67973100
C	-6.52134900	0.99525800	-0.16678700
C	-7.09257700	0.82618900	1.10740200
C	-7.32560600	1.57792100	-1.15845300
C	-8.40003200	1.22655700	1.38063200
H	-6.51598500	0.36528800	1.90415000
C	-8.63626000	1.98015700	-0.89006600
H	-6.93935200	1.72562900	-2.16136300
C	-9.18149600	1.80733600	0.38112000
H	-8.80727900	1.08125700	2.37760700
H	-9.22912800	2.42925200	-1.68249700
H	-10.20043600	2.12028400	0.59064900
C	-5.99748000	-1.66617400	-1.70869800
C	-5.46196300	-1.92921900	-2.90815000
H	-4.41034200	-1.76456300	-3.12287600
H	-6.05893700	-2.35419700	-3.71204400
C	-2.95054600	2.73616000	-2.84459700
H	-2.62070700	3.77783900	-2.82584500
H	-2.09631300	2.05685900	-2.73176500
H	-3.35255600	2.52005300	-3.84624900
C	-7.43943800	-2.00321900	-1.40568000
H	-7.49419600	-2.75063800	-0.60159400
H	-8.00869700	-1.13295300	-1.06270600
H	-7.94360900	-2.41873800	-2.28398500

TS-EF-5R-8

0 imaginary frequency

H = 0.000000

G = -5316.574116

E(M06-2X-DCM) = -5316.245286

O	1.02842600	-2.81743900	0.17948300
O	2.83393000	-1.00740900	-0.18704600
P	1.22146500	-1.20702600	-0.06720400
O	0.74695500	-0.38634200	1.09063100
C	2.83196300	-4.45081500	3.58807900
C	3.54381900	-4.31962700	2.40033800

C	2. 92145900	-3. 82995600	1. 24202900
C	0. 84991600	-3. 51927900	2. 49748700
C	1. 49007700	-4. 07223800	3. 61934000
C	3. 53266400	-1. 61961100	-1. 22969100
C	3. 87210100	-2. 96767300	-1. 13418500
C	4. 40500600	-3. 61537400	-2. 26024900
C	4. 71544900	-2. 89826400	-3. 41082600
C	4. 49326400	-1. 52054200	-3. 43293400
C	3. 88499200	-0. 85290600	-2. 35775900
H	0. 91929000	-4. 17895500	4. 53728500
H	4. 77084400	-0. 94158600	-4. 30885600
C	3. 87213600	-3. 92853800	0. 05320900
C	5. 24965200	-3. 87685000	0. 80140200
H	5. 50010000	-2. 82892900	1. 00270600
H	6. 06321600	-4. 30598300	0. 20862700
H	5. 59973900	-5. 38494000	-1. 86328300
H	4. 16404000	-5. 70735600	-2. 82875200
C	1. 60085400	-3. 39093500	1. 31360700
H	3. 31131600	-4. 83653700	4. 48431400
H	5. 13702300	-3. 39690400	-4. 28010500
C	5. 00310800	-4. 61501900	2. 13390700
H	5. 65776200	-4. 26494100	2. 94007600
H	5. 17832600	-5. 69541500	2. 03151800
C	4. 54702700	-5. 10040300	-2. 00028600
C	3. 73693000	-5. 29383200	-0. 69842400
H	2. 68063600	-5. 45939600	-0. 93962500
H	4. 07985400	-6. 13995500	-0. 09436200
C	3. 67124200	0. 62639600	-2. 41413900
C	2. 80294300	1. 18849600	-3. 38200100
C	4. 39267000	1. 46882200	-1. 53016600
C	2. 02949500	0. 39465900	-4. 28926200
C	2. 65817200	2. 62511100	-3. 46052800
C	4. 20980000	2. 90059400	-1. 59863000
C	1. 21503800	0. 97280600	-5. 22675100
H	2. 06727400	-0. 68419100	-4. 20364500
C	1. 79979900	3. 18812900	-4. 45678900
C	3. 35023100	3. 43908800	-2. 56021200
C	1. 10508400	2. 38899300	-5. 32378000
H	0. 62817500	0. 34346100	-5. 88966300
H	1. 71659500	4. 27157800	-4. 50903300
H	3. 21223300	4. 51685200	-2. 60305300
H	0. 45996800	2. 82891900	-6. 08023000
C	-0. 58408300	-3. 10527200	2. 61046500
C	-0. 93515400	-2. 01750700	3. 44662300

C	-1.59148500	-3.84853600	1.94881100
C	0.04041900	-1.19456100	4.09840100
C	-2.32865800	-1.69097100	3.64869400
C	-2.98072900	-3.50279100	2.14707100
C	-0.32827100	-0.14856100	4.90409500
H	1.09023600	-1.39687200	3.92545600
C	-2.67168100	-0.59965800	4.50919400
C	-3.31115800	-2.44453300	2.99917600
C	-1.70443200	0.15057800	5.12165200
H	0.43609900	0.46761800	5.37047100
H	-3.72561800	-0.37893300	4.66526200
H	-4.36068500	-2.20855000	3.16868100
H	-1.97969500	0.97865200	5.76930400
C	5.99608000	1.81016100	0.28530600
H	6.69463000	1.40033800	1.00979300
C	5.32678300	0.97035400	-0.56534600
H	5.50882000	-0.09687800	-0.51451800
C	5.78744400	3.21718100	0.23265300
H	6.32230900	3.86636900	0.92073500
C	4.92295400	3.74349400	-0.68833200
H	4.75290500	4.81496700	-0.74378200
C	-2.29740500	-5.66261100	0.47115900
H	-2.04590600	-6.49946400	-0.17473700
C	-3.66369300	-5.30957200	0.66013500
H	-4.44180300	-5.87844900	0.15828600
C	-3.99140200	-4.26320000	1.47953600
H	-5.03207300	-3.99127800	1.64116600
C	-1.30034100	-4.96157400	1.09693600
H	-0.26612900	-5.24960600	0.94819500
N	0.63253600	-0.94053700	-1.55318300
S	-0.86691500	-1.11695700	-1.98275200
O	-1.26883600	-0.15634600	-3.02540800
O	-1.83033300	-1.27829100	-0.85366100
C	-0.90414300	-2.76552800	-2.86877000
F	-0.00299300	-2.76529300	-3.85824600
F	-2.11978100	-2.96611900	-3.40122400
F	-0.63162200	-3.76644600	-2.03072100
C	-5.09517600	0.57760300	-0.42397100
C	-4.45132000	1.04945600	-1.75223600
H	-5.15800100	0.86356700	-2.57586500
H	-3.60249200	0.39743200	-1.97978600
C	-3.98011400	2.46612300	-1.91189300
C	-4.16115100	0.94298900	0.79244300
H	-4.50009500	1.85885800	1.27252900

H	-4. 22109100	0. 14033700	1. 53663100
N	-2. 74159300	1. 12727100	0. 47635700
C	-1. 98202200	2. 15397100	0. 91768500
N	-0. 65660800	1. 94421500	0. 98227300
C	0. 35055600	2. 89620700	1. 30762300
C	0. 47376600	4. 11593500	0. 63718500
C	1. 27291100	2. 54275400	2. 29552600
C	1. 49305000	4. 99615300	0. 99579000
C	2. 29361800	3. 43001500	2. 63692400
H	1. 18270500	1. 58218500	2. 78861000
C	2. 40436400	4. 66434900	2. 00017300
H	3. 18365100	5. 36081300	2. 28591400
C	3. 30237900	3. 03208900	3. 68309800
C	1. 64942800	6. 30348200	0. 26556300
F	2. 75919100	2. 21756400	4. 61758600
F	4. 35103000	2. 37249200	3. 14719000
F	3. 80194200	4. 11058900	4. 32806400
F	2. 02026100	7. 29820300	1. 10000300
F	2. 60539600	6. 23566600	-0. 69893900
F	0. 50893700	6. 68513100	-0. 34643800
S	-2. 69128700	3. 68423000	1. 33754600
H	-0. 22237700	4. 38050100	-0. 14694700
H	-0. 29313200	0. 96695800	0. 95994900
H	-2. 25179800	0. 28374300	0. 14643800
C	-4. 44228500	3. 54092000	-1. 14795200
H	-5. 40161200	3. 43509200	-0. 64386700
H	-3. 68347200	3. 57038000	-0. 11754700
H	-4. 24222500	4. 53876100	-1. 54242600
C	-5. 20479900	-0. 99802500	-0. 47031900
H	-5. 67767300	-1. 29963300	0. 47093500
H	-4. 18678000	-1. 40172800	-0. 45921200
C	-6. 50195500	1. 14915300	-0. 15886000
C	-7. 04648000	1. 08178500	1. 13647900
C	-7. 31922700	1. 67662900	-1. 16973300
C	-8. 33659300	1. 53364400	1. 41206800
H	-6. 46253200	0. 66230200	1. 95064600
C	-8. 61114900	2. 13370300	-0. 89900200
H	-6. 95821700	1. 74062500	-2. 19043800
C	-9. 12769500	2. 06609300	0. 39343200
H	-8. 72172700	1. 46780700	2. 42611000
H	-9. 21321300	2. 53942200	-1. 70768800
H	-10. 13261300	2. 42063900	0. 60462100
C	-5. 97316200	-1. 61181800	-1. 63189800
C	-7. 30796400	-1. 71328200	-1. 61660600

H	-7.90654200	-1.35379000	-0.78448500
H	-7.85050800	-2.17076500	-2.44079300
C	-2.92963000	2.68500700	-2.95048000
H	-2.58150400	3.72041600	-2.98004600
H	-2.08547200	1.99579200	-2.82102000
H	-3.34889600	2.43393800	-3.93687400
C	-5.15545500	-2.18032700	-2.76763000
H	-4.49071500	-1.43724400	-3.22381600
H	-4.49933100	-2.97984900	-2.40280700
H	-5.79629200	-2.59368700	-3.55316400

TS-EF-5R-9

l imaginary frequency

H = -5315.358555

G = -5315.558702

E(M06-2X-DCM) = -5316.241518

O	2.05584300	-2.38381100	-0.31934000
O	2.72598100	0.07410900	-0.75992500
P	1.43438800	-0.86892700	-0.42681400
O	0.83588000	-0.38890300	0.85490200
C	4.91887900	-3.03475600	2.67397700
C	5.28948000	-2.52470800	1.43466600
C	4.34338200	-2.37416000	0.40901400
C	2.59969000	-3.19099500	1.90845400
C	3.58769200	-3.38921000	2.88792700
C	3.45830000	-0.11381900	-1.93210800
C	4.41034500	-1.13053800	-1.98834800
C	5.02204400	-1.42872700	-3.21591300
C	4.78621800	-0.63849900	-4.33553000
C	3.93373500	0.45914400	-4.22092200
C	3.23881800	0.74008700	-3.03182700
H	3.28722800	-3.81063200	3.84274800
H	3.77650300	1.11133200	-5.07477000
C	5.04186000	-1.97723500	-0.88693100
C	6.31248600	-1.26504800	-0.30712100
H	6.04899900	-0.23285700	-0.04906500
H	7.13606300	-1.22887200	-1.02683800
H	6.96384000	-2.39245000	-3.10610300
H	5.73905200	-3.36827400	-3.90935300
C	3.00216100	-2.64786900	0.67271800
H	5.65189700	-3.15872200	3.46712400
H	5.26790600	-0.85902600	-5.28489300
C	6.65094900	-2.04985600	0.97755300
H	7.15530400	-1.43314500	1.73014500

H	7. 31820200	-2. 89729800	0. 76552300
C	5. 89731900	-2. 65747000	-3. 09009000
C	5. 47904300	-3. 22947400	-1. 71727700
H	4. 61353200	-3. 89088800	-1. 83848400
H	6. 27145500	-3. 80185400	-1. 22476800
C	2. 35503800	1. 94587500	-2. 97453500
C	1. 25172000	2. 05887200	-3. 85815600
C	2. 68654100	3. 02363600	-2. 11297900
C	0. 83560700	0. 99562600	-4. 72350300
C	0. 49178000	3. 28864500	-3. 90080200
C	1. 88406100	4. 22622300	-2. 13055600
C	-0. 20580300	1. 15241100	-5. 59971700
H	1. 34139600	0. 04055400	-4. 65558000
C	-0. 58158500	3. 41588500	-4. 83882100
C	0. 81990800	4. 33070200	-3. 03007800
C	-0. 91621400	2. 38380800	-5. 67406100
H	-0. 50587800	0. 32238800	-6. 23288300
H	-1. 11970700	4. 36092000	-4. 87759900
H	0. 24097700	5. 25217100	-3. 06049500
H	-1. 72760300	2. 49565200	-6. 38905100
C	1. 19099500	-3. 59149800	2. 21319100
C	0. 46982300	-2. 91547400	3. 22732500
C	0. 61947400	-4. 71036900	1. 55833500
C	0. 98531900	-1. 77042300	3. 91816300
C	-0. 84764700	-3. 38071200	3. 59777800
C	-0. 70649700	-5. 15212600	1. 92546400
C	0. 27161600	-1. 15420000	4. 91369900
H	1. 95681000	-1. 38152600	3. 63731500
C	-1. 55971600	-2. 70817600	4. 64093200
C	-1. 39924000	-4. 48132400	2. 93712300
C	-1. 01803400	-1. 63031200	5. 28690300
H	0. 69224200	-0. 28786900	5. 41595300
H	-2. 54599300	-3. 07935100	4. 91083700
H	-2. 38946000	-4. 83056900	3. 22306100
H	-1. 56784400	-1. 13077400	6. 08018600
C	4. 09394500	4. 05180600	-0. 39618400
H	4. 94998800	3. 99680200	0. 27093100
C	3. 81174400	2. 99926700	-1. 22701700
H	4. 45423000	2. 12711400	-1. 21859100
C	3. 27540500	5. 21636000	-0. 39161400
H	3. 49952100	6. 03441500	0. 28650300
C	2. 20627900	5. 29926200	-1. 24173700
H	1. 57290500	6. 18231400	-1. 25002100
C	0. 73455200	-6. 54388300	-0. 05444700

H	1.28484000	-7.09323600	-0.81366800
C	-0.58082800	-6.96062700	0.29592000
H	-1.02434000	-7.81954200	-0.20058300
C	-1.27538200	-6.28401600	1.26165800
H	-2.27622400	-6.59834500	1.54859400
C	1.31286200	-5.46212700	0.55618900
H	2.31852500	-5.16552500	0.28157000
N	0.56195500	-0.89346300	-1.79486500
S	-0.93139800	-1.35457800	-1.91551400
O	-1.68328600	-0.54730300	-2.89407100
O	-1.63098100	-1.60643300	-0.61994800
C	-0.86070300	-3.05706300	-2.67995400
F	-0.33553700	-2.99296700	-3.90752400
F	-2.10723600	-3.54909200	-2.76894600
F	-0.12408100	-3.87567300	-1.92934300
C	-5.22126900	-0.24608000	-0.51503700
C	-4.59550400	0.59477300	-1.67227500
H	-5.26825300	0.55906000	-2.54300700
H	-3.68117500	0.10568300	-2.02076700
C	-4.29309800	2.04588400	-1.47215400
C	-4.45167800	0.03472600	0.81948200
H	-4.94180100	0.82569000	1.38067500
H	-4.47932600	-0.86350300	1.44455600
N	-3.05478500	0.45222400	0.66704300
C	-2.47777200	1.46910400	1.34633900
N	-1.13151000	1.46909500	1.40289600
C	-0.28149400	2.47203300	1.94945400
C	-0.41508500	3.82840800	1.64507400
C	0.77541600	2.03903800	2.75700000
C	0.48088800	4.74815000	2.19065400
C	1.67044500	2.96831800	3.28213300
H	0.89264400	0.98150900	2.95503000
C	1.52349300	4.32948700	3.01553100
H	2.21766300	5.04979800	3.43228200
C	2.84724500	2.50379200	4.09881300
C	0.29280000	6.21602700	1.91569000
F	2.63951900	1.28374200	4.64729700
F	3.96952300	2.41452800	3.35193200
F	3.11789300	3.36004100	5.11009400
F	1.46782600	6.88664600	1.92596900
F	-0.28662600	6.43542100	0.71175600
F	-0.49894100	6.80257700	2.84174000
S	-3.43307100	2.73072500	2.06207300
H	-1.20119300	4.16724800	0.98512600

H	-0.60513300	0.61859800	1.12214800
H	-2.42739400	-0.24756400	0.23845000
C	-5.00397300	2.88039200	-0.59653400
H	-5.98917600	2.54743700	-0.27114700
H	-4.35435400	2.80851800	0.49343200
H	-4.92343200	3.95351000	-0.78142200
C	-5.04945900	-1.74765700	-0.97923500
H	-4.00705000	-1.88775000	-1.27778500
H	-5.65424900	-1.86570500	-1.88589700
C	-6.72946500	0.03632300	-0.32494200
C	-7.33107200	0.10348700	0.94246900
C	-7.57919300	0.15209600	-1.43981400
C	-8.70500400	0.31061800	1.08934300
H	-6.73989500	-0.02324300	1.84200500
C	-8.95100900	0.35727300	-1.29928500
H	-7.17854600	0.06801000	-2.44612300
C	-9.52339100	0.44506300	-0.02957400
H	-9.13121100	0.35845100	2.08777600
H	-9.57185100	0.44637500	-2.18683000
H	-10.59156500	0.60745500	0.08354300
C	-5.41215100	-2.84158000	0.01569500
C	-6.67918800	-3.20011000	0.25532800
H	-7.52145300	-2.72188400	-0.23562400
H	-6.91667600	-4.00072400	0.95215300
C	-3.15875500	2.59214700	-2.27197100
H	-2.91324400	3.62318300	-2.00583400
H	-2.27151500	1.95324600	-2.20158200
H	-3.43016000	2.56934800	-3.33852000
C	-4.25181700	-3.56824600	0.65518200
H	-3.62548800	-4.04339800	-0.11099100
H	-3.57849100	-2.89579200	1.20060800
H	-4.59848300	-4.34247600	1.34724700

TS-1-1-5S

l imaginary frequency

H = -5315.353570

G = -5315.550237

E(M06-2X-DCM) = -5316.238978

C	3.17955000	3.28005900	0.55756400
C	2.70515900	3.27984200	2.05879800
H	3.54190900	2.88900800	2.64681900
H	2.54418600	4.32741200	2.33736800
C	1.46074400	2.54320100	2.47505900
C	2.02409800	3.73233700	-0.37714900

H	2.39774200	3.79144500	-1.40524700
H	1.71068500	4.74137900	-0.10356100
N	0.83998200	2.88624900	-0.35771200
C	-0.40137600	3.36766100	-0.71506500
N	-1.28738200	2.34750500	-0.94498700
C	-2.61662300	2.32069600	-1.38996600
C	-3.51261900	3.40066500	-1.36929000
C	-3.06692900	1.07502200	-1.86374800
C	-4.81635600	3.22161500	-1.83388300
C	-4.37062200	0.91986400	-2.32276900
H	-2.38927900	0.22738700	-1.86737100
C	-5.26120800	1.99358600	-2.32139600
H	-6.27232400	1.87699100	-2.69203500
C	-4.84092400	-0.44329800	-2.74734900
C	-5.79742700	4.36004600	-1.72709300
F	-3.85923400	-1.16271900	-3.33963500
F	-5.87734100	-0.38383700	-3.60725000
F	-5.26173600	-1.18051100	-1.68058000
F	-5.19507200	5.56377600	-1.76074600
F	-6.49511500	4.30042000	-0.56156200
F	-6.71111700	4.32984600	-2.72285600
S	-0.74739300	5.01541000	-0.81284500
C	3.70728000	1.85639500	0.15150200
H	3.82686100	1.85587200	-0.93917300
H	2.92523400	1.12084800	0.36856200
H	-3.18735400	4.36332300	-1.00331800
C	1.50474100	1.24449900	2.99855200
H	-0.87917600	1.41139100	-0.85408700
H	0.67020200	0.97745700	3.65042000
H	0.98823100	1.89239400	-0.53449000
H	1.32883900	0.28198000	2.14893400
O	-1.35554200	-1.39549500	0.58027000
O	0.73238800	-2.51473600	-0.51266800
P	0.22193200	-1.16912500	0.23788800
O	0.28205000	0.06726300	-0.59910000
C	-2.52827700	-4.66061100	2.93151300
C	-2.17324900	-4.84289200	1.59995300
C	-1.88759400	-3.74224500	0.77757300
C	-2.24140900	-2.24420000	2.67520900
C	-2.60575300	-3.36550100	3.43987300
C	0.15939700	-2.82056500	-1.76271400
C	-1.05186600	-3.50676800	-1.78717700
C	-1.69962700	-3.69732100	-3.01873800
C	-1.10419200	-3.28695600	-4.20607800

C	0.15028400	-2.68057300	-4.16192600
C	0.80573400	-2.41785900	-2.94731300
H	-2.93366700	-3.20499600	4.46243300
H	0.63841600	-2.37764800	-5.08357700
C	-1.83029900	-4.20401200	-0.67682900
C	-1.35035000	-5.67967500	-0.47894400
H	-1.58558200	-6.31320700	-1.33998100
H	-0.26266800	-5.68085700	-0.34491800
H	-3.83262400	-3.86620400	-3.40824100
H	-3.02429800	-5.40776500	-3.11940100
C	-1.82280900	-2.47370400	1.34970400
H	-2.76170300	-5.51114800	3.56671600
H	-1.60519700	-3.43657700	-5.15889800
C	-2.03730900	-6.13675500	0.82681500
H	-3.01843000	-6.59004600	0.62837900
H	-1.44941700	-6.88416100	1.37133300
C	-3.04757100	-4.35097600	-2.81897100
C	-3.26954300	-4.19518600	-1.30072400
H	-3.91114400	-4.97065600	-0.87203300
H	-3.73983200	-3.22648000	-1.10301600
C	2.15732400	-1.77255000	-2.98909900
C	3.31156800	-2.55899000	-2.75317500
C	2.28677500	-0.41801600	-3.38032500
C	3.24788200	-3.95092400	-2.42529100
C	4.62143000	-1.96050800	-2.87654000
C	3.60423700	0.16068600	-3.52447900
C	4.38390000	-4.68590100	-2.20843700
H	2.27719500	-4.42755400	-2.34936100
C	5.78131300	-2.75972400	-2.63135300
C	4.73178200	-0.62086600	-3.25885700
C	5.67050100	-4.08401500	-2.30430400
H	4.30471200	-5.74052800	-1.95918100
H	6.75775900	-2.28918300	-2.71871700
H	5.72122600	-0.18091000	-3.36868500
H	6.55953600	-4.68189100	-2.12349100
C	-2.37708400	-0.88122600	3.28004000
C	-3.35487400	0.01580600	2.77805500
C	-1.61162300	-0.53034400	4.42160700
C	-4.21336600	-0.30099300	1.67690100
C	-3.53927600	1.30266000	3.41313000
C	-1.82939800	0.74806200	5.06433200
C	-5.14678900	0.59073100	1.21755100
H	-4.12670500	-1.27128400	1.20235700
C	-4.51066800	2.21255500	2.88845400

C	-2.77726500	1.63020000	4.53804500
C	-5.29017500	1.87445200	1.81611200
H	-5.77734000	0.31598000	0.37869400
H	-4.61582700	3.18348000	3.36689200
H	-2.93492500	2.59184700	5.02301300
H	-6.00737200	2.58076900	1.40911900
C	1.31823600	1.72638900	-4.05094700
H	0.44525000	2.34185100	-4.24955300
C	1.15983800	0.42479100	-3.65134100
H	0.16420500	0.01592400	-3.52934200
C	2.61962400	2.28575100	-4.20913900
H	2.72519300	3.31428900	-4.54393100
C	3.72693900	1.52261600	-3.94842200
H	4.72657900	1.93350700	-4.07232500
C	0.11914300	-1.01620300	6.08013200
H	0.89171500	-1.67820000	6.45957100
C	-0.11728400	0.23193000	6.72242900
H	0.45950700	0.50305400	7.60262900
C	-1.06203500	1.08819100	6.22319500
H	-1.25020900	2.04769000	6.69999000
C	-0.60211600	-1.38498800	4.97369700
H	-0.39157600	-2.33127000	4.49032700
N	1.16696300	-1.05978700	1.57605900
S	1.90171100	-2.25436600	2.42419100
C	3.29514300	-2.88778200	1.30468600
O	1.04685800	-3.42009800	2.65531600
O	2.59005800	-1.60443600	3.54357300
F	2.90818800	-3.99821000	0.68169700
F	3.64033900	-1.96290800	0.40656500
F	4.34865300	-3.16466600	2.07653300
C	4.29808300	4.33563400	0.37667500
C	4.76787800	4.63075500	-0.91730700
C	4.89787700	5.01773100	1.44512300
C	5.77200900	5.57267900	-1.13196900
H	4.36406400	4.10599300	-1.77726300
C	5.91018500	5.95803800	1.23459000
H	4.59687100	4.82130100	2.46755100
C	6.34994800	6.24605200	-0.05489600
H	6.10531200	5.77622300	-2.14617800
H	6.35182600	6.46402900	2.08896300
H	7.13340300	6.98044600	-0.21962700
C	5.01244400	1.38098300	0.78136200
H	2.47291900	0.89646700	3.35764900
C	0.18907100	3.32177600	2.57597500

H	0.11486700	4.14370200	1.86146100
H	-0.69344100	2.68008700	2.50580900
H	0.17669900	3.76006800	3.58788100
C	6.31399900	1.77696900	0.11915700
H	6.29496300	1.51589200	-0.94776600
H	6.50968200	2.85152000	0.17708300
H	7.15747700	1.25223000	0.57862800
C	5.02319200	0.55742800	1.83712700
H	5.95803300	0.19616300	2.25898200
H	4.12065400	0.17551900	2.30027100

TS-1-1-5S-1

l imaginary frequency

H = -5315.353238

G = -5315.550681

E(M06-2X-DCM) = -5316.237983

C	2.95226200	3.43933500	0.44610200
C	2.30517600	3.62547600	1.87077700
H	3.09528600	3.47477000	2.61145400
H	1.98222900	4.66993200	1.93225200
C	1.13855700	2.77621300	2.29811400
C	1.87923700	3.77230500	-0.63063600
H	2.34387200	3.72080700	-1.62262800
H	1.53003900	4.79747600	-0.49689500
N	0.71094400	2.90488000	-0.60027400
C	-0.54010300	3.32367400	-0.99611100
N	-1.39026000	2.26174800	-1.16430600
C	-2.72853600	2.16295800	-1.57062200
C	-3.66670300	3.20640400	-1.57066100
C	-3.14172800	0.87879000	-1.96912200
C	-4.97744100	2.95226400	-1.97700600
C	-4.45270300	0.64897800	-2.37259100
H	-2.42942300	0.06009800	-1.95745400
C	-5.38712100	1.68471500	-2.38860100
H	-6.40496600	1.50946800	-2.71508800
C	-4.87887500	-0.75148300	-2.71487800
C	-6.00144600	4.05351800	-1.88437500
F	-3.88861700	-1.45745200	-3.30897200
F	-5.94676200	-0.77650400	-3.53680000
F	-5.22894700	-1.45261700	-1.59933200
F	-5.45321200	5.27750900	-2.00364100
F	-6.64591900	4.02473200	-0.68742300
F	-6.95374500	3.93502600	-2.83611100
S	-0.94072400	4.94950100	-1.19875400

C	3.50937200	1.98651600	0.21574700
H	3.53585300	1.82002800	-0.86629900
H	2.78178900	1.26318200	0.60120700
H	-3.36917500	4.19855100	-1.26440600
C	1.31235700	1.51863500	2.89110000
H	-0.95252300	1.34649300	-1.01570200
H	0.50329500	1.20410200	3.55461400
H	0.88837000	1.90459400	-0.69864000
H	1.21893200	0.50847300	2.09468500
O	-1.30406800	-1.43192500	0.64179500
O	0.84029200	-2.48985400	-0.40957900
P	0.25191100	-1.13290400	0.26072300
O	0.22550200	0.04730800	-0.65579300
C	-2.28184700	-4.65686300	3.13497100
C	-1.93899200	-4.87180400	1.80497700
C	-1.71157700	-3.79007800	0.94089000
C	-2.10676600	-2.24007700	2.78743600
C	-2.40728100	-3.34884000	3.59790300
C	0.28522800	-2.88678600	-1.64326500
C	-0.90298600	-3.61298800	-1.63568500
C	-1.54683400	-3.87592400	-2.85602000
C	-0.96562600	-3.49975500	-4.06159700
C	0.27419300	-2.86238100	-4.04672600
C	0.92319200	-2.52867400	-2.84625400
H	-2.72705500	-3.16599500	4.61920900
H	0.75616800	-2.59247100	-4.98179400
C	-1.65124800	-4.29730500	-0.49728000
C	-1.11615200	-5.74809900	-0.25701200
H	-1.34106500	-6.41827400	-1.09259200
H	-0.02724200	-5.70675500	-0.14082900
H	-3.67551900	-4.12605000	-3.22601300
H	-2.81741000	-5.62968500	-2.88602700
C	-1.69839500	-2.49903700	1.46420300
H	-2.47055200	-5.49285800	3.80344800
H	-1.46373500	-3.70384100	-5.00579000
C	-1.76615400	-6.18526800	1.07390200
H	-2.73321000	-6.67953500	0.90658500
H	-1.14368100	-6.89262600	1.63331100
C	-2.87274200	-4.56389600	-2.62414800
C	-3.09290900	-4.35991700	-1.11103700
H	-3.70535800	-5.14068000	-0.65030800
H	-3.59507400	-3.40099800	-0.94587700
C	2.26906300	-1.87464500	-2.92003200
C	3.42804300	-2.64977000	-2.66844000

C	2.39003900	-0.53611500	-3.36388300
C	3.37237200	-4.03041600	-2.29347500
C	4.73462600	-2.05375200	-2.83079600
C	3.70415000	0.04029700	-3.54348200
C	4.51304800	-4.75559800	-2.06866100
H	2.40408900	-4.50646300	-2.18829500
C	5.89976300	-2.84167700	-2.57393900
C	4.83662700	-0.72909900	-3.26402400
C	5.79670400	-4.15454300	-2.20146800
H	4.44001000	-5.80174100	-1.78414700
H	6.87366900	-2.37218300	-2.69020400
H	5.82350200	-0.29231600	-3.40385100
H	6.68958700	-4.74414800	-2.01265900
C	-2.30159300	-0.86609300	3.34886300
C	-3.31578300	-0.02580200	2.82046200
C	-1.55677200	-0.45226200	4.48344800
C	-4.15078500	-0.40406600	1.72051300
C	-3.56316600	1.26512700	3.42571100
C	-1.84224500	0.82573100	5.10028800
C	-5.11421300	0.43782600	1.23007700
H	-4.02089700	-1.38096200	1.27031800
C	-4.56605900	2.12149700	2.87034900
C	-2.82882200	1.64949300	4.55112200
C	-5.31681800	1.72819700	1.79627100
H	-5.72422100	0.11718600	0.39244000
H	-4.71827900	3.09690400	3.32658800
H	-3.03676700	2.61147500	5.01613600
H	-6.05734900	2.39477500	1.36445200
C	1.40718800	1.57565700	-4.11160800
H	0.53027500	2.17894700	-4.32954200
C	1.25723500	0.28998300	-3.66011300
H	0.26485700	-0.11864600	-3.51390200
C	2.70506400	2.13440300	-4.29889900
H	2.80406900	3.15037600	-4.67163600
C	3.81773800	1.38609200	-4.01822400
H	4.81440800	1.79611400	-4.16663100
C	0.19354000	-0.81296800	6.15326600
H	1.00087400	-1.42415600	6.54532800
C	-0.11310800	0.43091100	6.77349200
H	0.44493100	0.74804900	7.65036200
C	-1.09965900	1.22662700	6.25586100
H	-1.33964000	2.18377400	6.71366300
C	-0.50306400	-1.24023200	5.05226800
H	-0.23749100	-2.18093700	4.58513200

N	1. 18689000	-0. 87234700	1. 58417300
S	2. 05866600	-1. 93347200	2. 47447600
C	3. 53128800	-2. 40463000	1. 38340500
O	1. 35639500	-3. 19022800	2. 73834100
O	2. 65228100	-1. 16732000	3. 57482600
F	3. 28466800	-3. 54403800	0. 74480400
F	3. 78832300	-1. 43743000	0. 49705300
F	4. 59512600	-2. 56656800	2. 17378800
C	4. 07677000	4. 48042400	0. 24893700
C	4. 76728900	4. 51022700	-0. 97663400
C	4. 44730500	5. 42318400	1. 21780800
C	5. 77011000	5. 44416700	-1. 22444500
H	4. 52678600	3. 78883300	-1. 75127000
C	5. 45726500	6. 35873000	0. 97496600
H	3. 95757000	5. 44950800	2. 18476700
C	6. 12193900	6. 37739300	-0. 24787000
H	6. 28064500	5. 43888400	-2. 18388300
H	5. 71719800	7. 07444400	1. 75038500
H	6. 90472800	7. 10624100	-0. 43876400
C	4. 88712300	1. 63742300	0. 76011300
H	2. 30743400	1. 28515200	3. 26834200
C	-0. 21403200	3. 40819100	2. 31368200
H	-0. 35367300	4. 16153300	1. 53551800
H	-1. 01762600	2. 66777800	2. 27759600
H	-0. 30502500	3. 92056500	3. 28602700
C	5. 10860800	1. 57066800	2. 25268300
H	4. 96810000	2. 54520800	2. 73782300
H	4. 42379900	0. 85800600	2. 73015900
H	6. 12869600	1. 24513600	2. 47823500
C	5. 87815700	1. 32692100	-0. 08244500
H	6. 86185800	1. 03700800	0. 27857500
H	5. 74175500	1. 33815200	-1. 15987900

TS-1-1-5S-2

l imaginary frequency

H = -5315. 341406

G = -5315. 540354

E(M06-2X-DCM) = -5316. 225665

C	-4. 39594200	2. 17963400	0. 57164700
C	-3. 72784600	2. 40079300	1. 99659900
H	-4. 35041800	1. 85990100	2. 71468700
H	-3. 82153500	3. 47128000	2. 21467000
C	-2. 29751000	2. 01627700	2. 24128600
C	-3. 62073400	2. 94283100	-0. 52517000

H	-4.18502500	2.88704400	-1.46482300
H	-3.53265300	3.99913600	-0.27054000
N	-2.26570000	2.45385400	-0.73089800
C	-1.26417900	3.25019300	-1.25937600
N	-0.12229600	2.52668700	-1.45795200
C	1.14659300	2.86530200	-1.96163300
C	1.65369300	4.16106500	-2.10742600
C	1.97284100	1.76937900	-2.27865700
C	2.97278400	4.33966800	-2.53803700
C	3.27738300	1.97026800	-2.71023500
H	1.58678700	0.76318900	-2.17094200
C	3.79770700	3.26156700	-2.84209700
H	4.81969000	3.41945700	-3.16534200
C	4.13550400	0.79168600	-3.08165500
C	3.52573800	5.73974400	-2.55430600
F	3.63824000	-0.37533400	-2.60816900
F	4.24371900	0.65180900	-4.42682100
F	5.39552900	0.91199100	-2.60522700
F	4.65696400	5.83595100	-3.28506400
F	2.64210000	6.62970700	-3.04876400
F	3.83304200	6.15311200	-1.29591100
S	-1.47587600	4.89254600	-1.55895600
H	1.03182000	5.01374200	-1.87398400
C	-1.96435000	0.76737300	2.78673100
H	-0.09940800	1.61068400	-0.99398300
H	-2.77437300	0.20111600	3.24908100
H	-1.01951300	0.73647800	3.33458400
H	-2.20210300	1.47096200	-0.97366800
H	-1.63233000	-0.07865100	1.89001200
O	1.40804100	-1.57404300	1.65779600
O	0.64804500	-1.82260000	-0.83498500
P	0.34578000	-1.02783000	0.55129000
O	0.46004500	0.42741600	0.24982600
C	5.40190900	-0.47886700	1.00591300
C	4.85533300	-1.58789900	0.37015200
C	3.54687300	-2.00306200	0.65979800
C	3.29433000	-0.12887400	2.20450200
C	4.63316900	0.21210200	1.94063500
C	0.81918500	-3.20325500	-1.02586300
C	1.91578400	-3.86057200	-0.46415300
C	1.94024600	-5.26488800	-0.47555800
C	0.98425400	-5.98662700	-1.17944400
C	0.02334900	-5.29240200	-1.90887000
C	-0.09363300	-3.89161000	-1.85194400

H	5.06184400	1.05512100	2.47385300
H	-0.67274800	-5.83789800	-2.53762300
C	3.27460600	-3.35756800	0.02530900
C	4.28228000	-3.30899100	-1.17801600
H	4.55543000	-4.30828900	-1.52873300
H	3.81163300	-2.78092500	-2.01263200
H	3.87145000	-6.24725800	-0.35366200
H	2.83048200	-6.56367900	1.02920300
C	2.76188700	-1.23020400	1.50711400
H	6.41757700	-0.15792100	0.79004500
H	1.00958800	-7.07306000	-1.20183200
C	5.48557300	-2.48834100	-0.66680800
H	5.96934000	-1.91456800	-1.46511700
H	6.25690500	-3.13125100	-0.22056200
C	3.12290500	-5.79111500	0.30868000
C	3.67053500	-4.52035100	0.99252000
H	3.16516700	-4.36629300	1.95305500
H	4.74822100	-4.55567300	1.18069800
C	-1.08974000	-3.24506200	-2.76493300
C	-2.45220600	-3.64617000	-2.72070600
C	-0.63885200	-2.38488200	-3.80433800
C	-2.99014100	-4.45635600	-1.66768700
C	-3.35716200	-3.23169100	-3.76952600
C	-1.57300400	-1.93763300	-4.81493300
C	-4.30211400	-4.85458200	-1.67432300
H	-2.35295400	-4.72599400	-0.83557400
C	-4.71432000	-3.68262700	-3.74540300
C	-2.89404300	-2.39099300	-4.78400300
C	-5.17630400	-4.47770200	-2.73227000
H	-4.68304200	-5.45584000	-0.85338000
H	-5.37302200	-3.37122700	-4.55308500
H	-3.57901200	-2.07991900	-5.57075000
H	-6.21053200	-4.81145500	-2.72317100
C	2.55118600	0.65593400	3.23832000
C	2.36065100	2.05057100	3.06079900
C	2.16381400	0.03443000	4.45378300
C	2.70324100	2.73699000	1.84884200
C	1.79923400	2.83770200	4.13666900
C	1.55196300	0.82665700	5.49792700
C	2.55897300	4.09602300	1.72922100
H	3.07313000	2.16085000	1.00932300
C	1.66849300	4.25358700	3.97313400
C	1.39606200	2.20378600	5.31519200
C	2.04620600	4.86920500	2.81010800

H	2.83617800	4.59222400	0.80352900
H	1.26562200	4.83145300	4.80213500
H	0.96728800	2.79969500	6.11881100
H	1.94809100	5.94569000	2.70077000
C	1.11500200	-1.11726800	-4.95481500
H	2.15196100	-0.80194100	-5.01902600
C	0.72137000	-1.95534500	-3.94314700
H	1.46122200	-2.30306900	-3.23378600
C	0.17938700	-0.65350800	-5.92176900
H	0.50768500	0.01371600	-6.71391000
C	-1.12382300	-1.06289400	-5.85389100
H	-1.84914500	-0.73300200	-6.59406900
C	1.99764800	-1.92202200	5.91125000
H	2.17845200	-2.97906500	6.08608300
C	1.36096800	-1.14421000	6.91907700
H	1.05535400	-1.61375700	7.85003100
C	1.15078800	0.19238700	6.71567400
H	0.68308200	0.80428700	7.48350600
C	2.38631300	-1.35361200	4.72660500
H	2.87743500	-1.96388800	3.97831200
N	-1.12760100	-1.32714300	1.23115600
S	-1.78411300	-2.68371700	1.85210200
C	-1.00385900	-2.91348300	3.54935500
O	-3.18495900	-2.37747900	2.14746300
O	-1.40354200	-3.89262200	1.11935400
F	-1.77521100	-3.74381500	4.25615300
F	-0.92989400	-1.73956600	4.19354300
F	0.21708000	-3.43803900	3.44768300
C	-1.23486500	3.04656200	2.07399000
H	-0.30407200	2.60217100	1.70955800
H	-1.53054800	3.87897300	1.43432100
H	-1.01014600	3.45022200	3.07350600
C	-5.81708200	2.77603000	0.72039600
C	-6.74691200	2.16296600	1.57842600
C	-6.22014000	3.95312500	0.06973400
C	-8.02279100	2.68989500	1.76936100
H	-6.48129600	1.25409000	2.11080500
C	-7.50025700	4.48213800	0.25607100
H	-5.54901300	4.47615700	-0.60143500
C	-8.40895800	3.85487300	1.10510400
H	-8.71536200	2.18574000	2.43807600
H	-7.78014900	5.39151100	-0.26887000
H	-9.40368300	4.26714200	1.24948200
C	-4.44386800	0.64795400	0.25699900

H	-3.45422200	0.21743100	0.43496700
H	-5.10217000	0.15620800	0.98292900
C	-4.87307700	0.27470000	-1.15067900
C	-3.99800500	-0.29306000	-1.98831300
H	-2.98021200	-0.53734600	-1.69099000
H	-4.27780000	-0.58829900	-2.99382700
C	-6.30702900	0.50718800	-1.56498700
H	-6.99866500	0.03472000	-0.85528300
H	-6.56999400	1.57062000	-1.58834000
H	-6.49723300	0.08677200	-2.55708800

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l imaginary frequency

H = -5315.354732

G = -5315.551664

E(M06-2X-DCM) = -5316.238394

C	2.05048000	4.36338800	0.85587000
C	1.04091600	4.14699700	2.04109200
H	1.53926100	4.50152900	2.95506800
H	0.19077200	4.81151100	1.85991300
C	0.50648600	2.77879600	2.38970300
C	1.28383400	4.18476300	-0.48425000
H	1.99024400	4.07548500	-1.31296900
H	0.71976600	5.09771500	-0.67341500
N	0.31283800	3.10063800	-0.52755200
C	-1.00655500	3.28791600	-0.87234600
N	-1.62804500	2.09767800	-1.14459400
C	-2.93038000	1.75935800	-1.54062900
C	-4.05069500	2.60409300	-1.51023200
C	-3.09454900	0.43269300	-1.98093300
C	-5.29065500	2.11820700	-1.92785700
C	-4.33832600	-0.02767800	-2.39882200
H	-2.24058800	-0.23675600	-1.99223000
C	-5.45289500	0.81131900	-2.38426400
H	-6.41905200	0.45761800	-2.72316400
C	-4.49376100	-1.46905000	-2.79684800
C	-6.50521900	3.00195800	-1.80780400
F	-3.37819000	-1.96307100	-3.38163400
F	-5.51904000	-1.65621500	-3.65182300
F	-4.74007700	-2.26279400	-1.71562100
F	-6.19778400	4.31131600	-1.87382000
F	-7.14122800	2.80478800	-0.62310700
F	-7.41075700	2.74345400	-2.77778100
S	-1.74444300	4.80797300	-0.89697600

H	-3.94643400	3.62527000	-1.17461300
C	1.29263300	1.71723600	2.84904600
H	-1.01689800	1.27867100	-1.06113000
H	0.79244600	1.08713400	3.59270100
H	0.67291800	2.15280800	-0.63821700
H	1.34907900	0.68817200	2.03626400
O	-0.93201100	-1.57037300	0.56174200
O	1.35192800	-2.22291200	-0.52843500
P	0.55780700	-1.00814400	0.19907000
O	0.34188300	0.19285700	-0.66286200
C	-1.35479200	-4.98677400	2.95756600
C	-0.96027500	-5.10125700	1.63006300
C	-0.92852000	-3.97636300	0.79152400
C	-1.63678400	-2.57305900	2.66093600
C	-1.73586300	-3.73811800	3.44172600
C	0.86752500	-2.67405800	-1.77101200
C	-0.16287300	-3.60948000	-1.78099700
C	-0.74592900	-3.96759700	-3.00727300
C	-0.24776800	-3.46530300	-4.20405500
C	0.84404800	-2.59909200	-4.17341300
C	1.41846700	-2.17072700	-2.96485900
H	-2.10342300	-3.64283200	4.45883900
H	1.26073900	-2.21938500	-5.10168600
C	-0.76662700	-4.43945600	-0.65531300
C	0.03544500	-5.76402600	-0.43450500
H	-0.04798600	-6.44817800	-1.28481600
H	1.09463100	-5.51524900	-0.30263800
H	-2.78751200	-4.61369000	-3.38802300
H	-1.65772700	-5.93092300	-3.07046500
C	-1.15690400	-2.71611500	1.34351800
H	-1.38952100	-5.85842800	3.60589500
H	-0.69741000	-3.74404600	-5.15346700
C	-0.53175300	-6.34309100	0.87939700
H	-1.38352500	-7.01123300	0.69087900
H	0.20956600	-6.92736900	1.43604900
C	-1.91562400	-4.89995900	-2.79093000
C	-2.16980500	-4.76713200	-1.27533900
H	-2.62200300	-5.65784200	-0.82936700
H	-2.84563800	-3.92472000	-1.09626500
C	2.59660300	-1.24784900	-3.02199100
C	3.89354700	-1.75651300	-2.76718000
C	2.42627400	0.09369500	-3.44090500
C	4.13350300	-3.11676000	-2.39102900
C	5.04197100	-0.89155400	-2.91802500

C	3.58399500	0.94673200	-3.59270400
C	5.40194000	-3.58022600	-2.15853300
H	3.28923100	-3.78915000	-2.29015600
C	6.34870900	-1.41364000	-2.66166500
C	4.85639300	0.43294000	-3.32590700
C	6.52773200	-2.71857400	-2.28972000
H	5.55335400	-4.61715900	-1.87147200
H	7.20049300	-0.74727200	-2.77670500
H	5.72498000	1.07708800	-3.44877700
H	7.52574600	-3.10394300	-2.09988400
C	-2.12530400	-1.28969300	3.26188700
C	-3.30752400	-0.68264600	2.76202100
C	-1.50338800	-0.77344300	4.42838800
C	-4.01193900	-1.16957800	1.61455600
C	-3.86888500	0.46204400	3.44743900
C	-2.09469600	0.35180500	5.11973200
C	-5.14490700	-0.55102100	1.15476900
H	-3.64038400	-2.04737300	1.09971900
C	-5.04503400	1.08673600	2.92484200
C	-3.25940500	0.93457400	4.61300400
C	-5.66345900	0.60488400	1.80365900
H	-5.64700000	-0.94521900	0.27793000
H	-5.43496400	1.96036900	3.44194500
H	-3.70228600	1.77969600	5.13696300
H	-6.53803000	1.10340400	1.39663800
C	1.01085300	1.96342000	-4.13508300
H	0.02432900	2.36876700	-4.34202300
C	1.14212600	0.66170700	-3.72671600
H	0.26165400	0.04230300	-3.60622900
C	2.15598100	2.79839900	-4.28562200
H	2.03204300	3.82686100	-4.61329900
C	3.40364600	2.30099100	-4.01923300
H	4.28620800	2.92637900	-4.13157600
C	0.29141300	-0.79121300	6.08992500
H	1.22577900	-1.20885200	6.45295200
C	-0.30901800	0.30021200	6.77938700
H	0.15954200	0.69382800	7.67739600
C	-1.46760600	0.85339300	6.30378900
H	-1.93511100	1.69098100	6.81684700
C	-0.28741300	-1.31385500	4.96135600
H	0.19121000	-2.13916100	4.44822100
N	1.46293000	-0.66143000	1.52336700
S	2.39928200	-1.65596100	2.42960600
C	3.89991400	-2.07404700	1.35149600

O	1. 77666600	-2. 95476700	2. 69739100
O	2. 92751300	-0. 84500900	3. 52753400
F	3. 72648800	-3. 25746100	0. 76637600
F	4. 09333700	-1. 13975800	0. 41795400
F	4. 97385900	-2. 13248700	2. 14279600
H	2. 34392500	1. 90032800	3. 05469200
C	-0. 98046200	2. 64906500	2. 45430100
H	-1. 48776400	3. 25207400	1. 69769100
H	-1. 30811500	1. 60849100	2. 40115000
H	-1. 30325000	3. 03109900	3. 43530300
C	3. 29875400	3. 48153900	1. 01821600
C	3. 68928400	2. 52711700	0. 07096100
C	4. 11543400	3. 63875400	2. 15406900
C	4. 85561900	1. 77397600	0. 23963900
H	3. 09865500	2. 35542800	-0. 82244300
C	5. 27191700	2. 88363700	2. 33204500
H	3. 84775100	4. 36165400	2. 92062600
C	5. 65159700	1. 94685300	1. 36859500
H	5. 12659800	1. 04398200	-0. 51533400
H	5. 87613500	3. 02773100	3. 22379000
H	6. 55228400	1. 35458700	1. 50280700
C	2. 44829700	5. 88796100	0. 93177300
H	3. 02354500	6. 04957600	1. 85204300
H	1. 51650900	6. 45477800	1. 04116000
C	3. 22203100	6. 47060300	-0. 23893500
C	2. 62276500	7. 31085000	-1. 09166400
H	1. 57340300	7. 57888700	-0. 99639000
H	3. 16406700	7. 76395100	-1. 91881400
C	4. 68901300	6. 13468100	-0. 37271600
H	4. 85076600	5. 07013100	-0. 57414000
H	5. 14985700	6. 70998500	-1. 18184100
H	5. 22993200	6. 35790800	0. 55650400

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l imaginary frequency

H = -5315. 352866

G = -5315. 550096

E(M06-2X-DCM) = -5316. 237056

C	2. 00494700	4. 36274400	0. 94849200
C	1. 00933900	4. 13980700	2. 14444500
H	1. 52943500	4. 45441300	3. 05996100
H	0. 17430800	4. 83137900	1. 99560200
C	0. 44465500	2. 77395300	2. 45223400
C	1. 21168700	4. 23618800	-0. 37853500

H	1.90460800	4.20211600	-1.22626000
H	0.60611900	5.13520200	-0.49201000
N	0.27217400	3.12786500	-0.46495500
C	-1.04352400	3.29340100	-0.83830000
N	-1.64150400	2.09476200	-1.12064500
C	-2.93364900	1.73777300	-1.53456800
C	-4.06853100	2.56289900	-1.50766600
C	-3.07119200	0.41171300	-1.98555000
C	-5.29636100	2.05928300	-1.93979600
C	-4.30347200	-0.06671500	-2.41727100
H	-2.20605100	-0.24318700	-1.99306000
C	-5.43218600	0.75316300	-2.40678400
H	-6.38924500	0.38538900	-2.75637300
C	-4.43176700	-1.50795700	-2.82540800
C	-6.52687500	2.92115100	-1.82327500
F	-3.30332700	-1.98032900	-3.40279900
F	-5.44622000	-1.70624700	-3.69084100
F	-4.67535700	-2.31186800	-1.75109500
F	-6.24144400	4.23605300	-1.87753200
F	-7.16864500	2.70459100	-0.64507900
F	-7.42012400	2.65416800	-2.80223500
S	-1.80396800	4.80235400	-0.88498400
H	-3.98523500	3.58294900	-1.16308500
C	1.20861100	1.69459800	2.90872800
H	-1.01890900	1.28459200	-1.03027100
H	0.68063900	1.04873600	3.61850500
H	0.65702100	2.19042700	-0.58241300
H	1.30755900	0.69154200	2.07224600
O	-0.91017800	-1.58424300	0.55458100
O	1.38572700	-2.18906100	-0.53696900
P	0.57201300	-0.99450400	0.20237000
O	0.33977800	0.21263400	-0.64676700
C	-1.27764800	-5.01943700	2.93301100
C	-0.87733800	-5.12012500	1.60615100
C	-0.86456100	-3.99072300	0.77327600
C	-1.60216100	-2.60966300	2.64733500
C	-1.68273600	-3.78029500	3.42201900
C	0.90741200	-2.64083900	-1.78182400
C	-0.10482300	-3.59620400	-1.79649700
C	-0.68169500	-3.95907200	-3.02428900
C	-0.19518500	-3.44038200	-4.21873500
C	0.87910900	-2.55308100	-4.18399200
C	1.44679000	-2.12049300	-2.97360800
H	-2.05478500	-3.69675100	4.43852100

H	1. 28731600	-2. 15983300	-5. 11037300
C	-0. 69228400	-4. 44368000	-0. 67523800
C	0. 13475000	-5. 75361700	-0. 45980500
H	0. 06572000	-6. 43512600	-1. 31352900
H	1. 18874000	-5. 48514100	-0. 32498400
H	-2. 70993700	-4. 64335600	-3. 40869300
H	-1. 55447200	-5. 93968200	-3. 09756100
C	-1. 11679200	-2. 73742700	1. 33036500
H	-1. 29824000	-5. 89468400	3. 57708500
H	-0. 64037500	-3. 72256600	-5. 16922100
C	-0. 42334500	-6. 34980900	0. 85041600
H	-1. 26144600	-7. 03372900	0. 65728900
H	0. 32836900	-6. 92192300	1. 40575900
C	-1. 83261800	-4. 91541600	-2. 81284200
C	-2. 08908300	-4. 79512200	-1. 29681100
H	-2. 52434700	-5. 69632700	-0. 85510200
H	-2. 78050200	-3. 96632300	-1. 11366300
C	2. 60784100	-1. 17627000	-3. 03262900
C	3. 91548100	-1. 66345500	-2. 79099700
C	2. 41090200	0. 16250900	-3. 44864600
C	4. 18133200	-3. 01817100	-2. 41215500
C	5. 04821700	-0. 78125500	-2. 95952700
C	3. 55284600	1. 03357100	-3. 61591800
C	5. 45964800	-3. 46063500	-2. 19328600
H	3. 34906200	-3. 70315900	-2. 29746600
C	6. 36613600	-1. 28204800	-2. 71840100
C	4. 83673600	0. 53913600	-3. 36827800
C	6. 57016200	-2. 58232100	-2. 34307300
H	5. 63077800	-4. 49362000	-1. 90307300
H	7. 20586300	-0. 60294800	-2. 84680500
H	5. 69350900	1. 19628100	-3. 50454000
H	7. 57639300	-2. 95126700	-2. 16428700
C	-2. 11306100	-1. 33796200	3. 25378500
C	-3. 30025400	-0. 74350100	2. 75047300
C	-1. 50577500	-0. 82162700	4. 42794700
C	-3. 99038600	-1. 23160500	1. 59482000
C	-3. 88188200	0. 38827900	3. 44044600
C	-2. 11727400	0. 29012200	5. 12367900
C	-5. 12828600	-0. 62488400	1. 13147600
H	-3. 60372200	-2. 10064400	1. 07636000
C	-5. 06285200	1. 00083100	2. 91425300
C	-3. 28674600	0. 86040700	4. 61358600
C	-5. 66681900	0. 51915500	1. 78511400
H	-5. 61894900	-1. 01939700	0. 24830200

H	-5.46829800	1.86511500	3.43512800
H	-3.74497800	1.69509800	5.14106900
H	-6.54519600	1.00885400	1.37555200
C	0.95680900	2.01011700	-4.12162400
H	-0.03875900	2.39988700	-4.31480600
C	1.11424100	0.71012000	-3.71703900
H	0.24544200	0.07655200	-3.58602600
C	2.08649500	2.86316900	-4.28635000
H	1.94197000	3.88975700	-4.61167300
C	3.34547600	2.38527300	-4.03819500
H	4.21636000	3.02483400	-4.16091000
C	0.27810600	-0.82696700	6.10146800
H	1.21597200	-1.23401900	6.46750100
C	-0.34255800	0.25011800	6.79547000
H	0.11412100	0.64300200	7.69989400
C	-1.50533800	0.79101200	6.31598200
H	-1.98802400	1.61790400	6.83232500
C	-0.28538000	-1.34861300	4.96471200
H	0.20913800	-2.16231300	4.44804000
N	1.46598600	-0.64809700	1.53353500
S	2.42030400	-1.63478000	2.42935600
C	3.92482100	-2.02075000	1.34334000
O	1.81890300	-2.94544600	2.68850300
O	2.93734300	-0.82470600	3.53331400
F	3.77138300	-3.20644100	0.75642500
F	4.09701900	-1.08188600	0.41124300
F	5.00272900	-2.06081300	2.13065700
H	2.25339900	1.86737800	3.15361200
C	-1.04476100	2.66203200	2.47900000
H	-1.52856000	3.29887000	1.73490600
H	-1.38449200	1.62849900	2.38079700
H	-1.38276900	3.01030100	3.46753500
C	3.24014800	3.45629600	1.06341000
C	3.64820400	2.58801100	0.04543000
C	4.03975300	3.51941600	2.22056300
C	4.80787400	1.81704000	0.17301200
H	3.07676600	2.49806000	-0.87200500
C	5.19141600	2.74853700	2.35611700
H	3.76405200	4.18263900	3.03697800
C	5.58318200	1.89037600	1.32623200
H	5.09014200	1.15078600	-0.63494400
H	5.78074400	2.81724900	3.26657200
H	6.47774500	1.28250700	1.42769200
C	2.46128000	5.86919900	1.05728600

H	3.03846300	5.97973400	1.98051900
H	1.55581500	6.47709300	1.18191200
C	3.27408900	6.42731100	-0.10614900
C	4.59058400	6.21270100	-0.21061800
H	5.14094200	5.62076600	0.51443800
H	5.16526700	6.62585000	-1.03622600
C	2.53999700	7.29384300	-1.10411700
H	2.08690700	8.16180500	-0.60541600
H	3.21551200	7.66624100	-1.88053000
H	1.71896300	6.75959100	-1.59752800

TS-1-1-5R-2

l imaginary frequency

H = -5315.349490

G = -5315.547237

E(M06-2X-DCM) = -5316.231959

C	2.22610500	4.28735600	-0.62052000
C	1.29967500	4.52438100	0.61915000
H	1.88774500	5.04426900	1.38412500
H	0.50878300	5.21114300	0.30096400
C	0.65963200	3.36364300	1.34569500
C	1.33367000	3.77650700	-1.79230100
H	1.96376800	3.41589600	-2.61269600
H	0.77110800	4.62690900	-2.17843100
N	0.33808400	2.76970500	-1.46178400
C	-0.99108000	2.89635300	-1.81091700
N	-1.65937000	1.70969600	-1.68275100
C	-2.99038700	1.32479100	-1.90360500
C	-4.08558300	2.18739600	-2.06296800
C	-3.21226500	-0.06465200	-1.93041400
C	-5.35993200	1.65239200	-2.25776000
C	-4.48991300	-0.57532300	-2.13138800
H	-2.37669000	-0.74234100	-1.78940700
C	-5.58077500	0.27694900	-2.30484200
H	-6.57408900	-0.11998200	-2.47586500
C	-4.70398900	-2.06274500	-2.08173900
C	-6.54355000	2.58139900	-2.33822800
F	-3.63864200	-2.75070600	-2.55272100
F	-5.78400700	-2.44794400	-2.79066900
F	-4.90295800	-2.49671700	-0.80440000
F	-6.20859800	3.80357000	-2.79380100
F	-7.11378700	2.75756000	-1.11729700
F	-7.51019700	2.09241700	-3.14689800
S	-1.68164200	4.36296200	-2.28741500

H	-3.93700900	3.25690200	-2.04400700
C	1.37327400	2.40526400	2.07385400
H	-1.06707500	0.92513700	-1.38864300
H	0.84298000	2.04142000	2.95999600
H	0.67035500	1.81648300	-1.31114900
H	1.39568000	1.18955700	1.57557600
O	-0.95191600	-1.33608700	0.96324300
O	1.24935700	-2.36193200	-0.00416700
P	0.51876200	-0.95850500	0.36150700
O	0.26273600	-0.07517800	-0.81620500
C	-1.26325000	-3.86731400	4.29335300
C	-0.96456200	-4.38543300	3.03889200
C	-0.96929800	-3.56114400	1.90338000
C	-1.52008100	-1.64070100	3.30772400
C	-1.58530000	-2.51734900	4.40527100
C	0.67763800	-3.14335100	-1.02757700
C	-0.37153800	-3.99802900	-0.70110200
C	-1.04400100	-4.67643400	-1.73040500
C	-0.61656900	-4.56943100	-3.04883600
C	0.49483500	-3.77965300	-3.33841300
C	1.15908000	-3.03846200	-2.34649100
H	-1.87865900	-2.11067800	5.36819100
H	0.85749400	-3.70838000	-4.35961700
C	-0.91680500	-4.43543600	0.65240100
C	-0.13186800	-5.66921200	1.20789400
H	-0.29147600	-6.56947900	0.60617000
H	0.93949900	-5.43890900	1.19453300
H	-3.12112100	-5.31901000	-1.78480600
H	-2.00371700	-6.53148800	-1.15723500
C	-1.13735900	-2.18644500	2.06616900
H	-1.27007400	-4.50567400	5.17300000
H	-1.13554100	-5.09566900	-3.84570400
C	-0.61682200	-5.81013100	2.66679300
H	-1.49424800	-6.46780000	2.73818400
H	0.14923200	-6.23464800	3.32539800
C	-2.21785900	-5.45391500	-1.18091100
C	-2.36594600	-4.87107500	0.23946600
H	-2.80770400	-5.57126400	0.95459200
H	-3.00795700	-3.98509300	0.19963300
C	2.35483100	-2.23052700	-2.74777900
C	3.65208300	-2.70599000	-2.43643200
C	2.19222000	-1.06943500	-3.54127100
C	3.88033000	-3.89872900	-1.67830200
C	4.81029900	-1.99005700	-2.92181100

C	3. 35925100	-0. 36525500	-4. 02385300
C	5. 14878000	-4. 33648000	-1. 40057300
H	3. 02712600	-4. 46261200	-1. 31890600
C	6. 11697600	-2. 47913200	-2. 60726900
C	4. 63278100	-0. 84375600	-3. 70250100
C	6. 28588300	-3. 61704500	-1. 86578300
H	5. 29142700	-5. 24337400	-0. 81940900
H	6. 97648000	-1. 92540700	-2. 97802400
H	5. 50790800	-0. 31634200	-4. 07751100
H	7. 28383200	-3. 97923600	-1. 63450300
C	-1. 94028800	-0. 21902300	3. 52637300
C	-3. 13758000	0. 26188900	2. 93394800
C	-1. 23232100	0. 59218900	4. 45085900
C	-3. 92630000	-0. 51253500	2. 02374800
C	-3. 62642900	1. 58038100	3. 27730200
C	-1. 75079700	1. 89550000	4. 80674400
C	-5. 07131900	-0. 01062800	1. 46280500
H	-3. 61038800	-1. 51835900	1. 77447800
C	-4. 81879000	2. 07128200	2. 65746300
C	-2. 93168500	2. 35052700	4. 21403300
C	-5. 51941800	1. 30606600	1. 76567000
H	-5. 63786400	-0. 62505600	0. 77151400
H	-5. 15390800	3. 07408800	2. 91198600
H	-3. 31943800	3. 33062500	4. 48600500
H	-6. 40636100	1. 69821300	1. 27712000
C	0. 78256800	0. 57780000	-4. 67300700
H	-0. 20476100	0. 95395300	-4. 92616800
C	0. 90706600	-0. 54650700	-3. 89911300
H	0. 02108500	-1. 05345300	-3. 53695400
C	1. 93665600	1. 26642700	-5. 14732700
H	1. 81781500	2. 15282300	-5. 76450500
C	3. 18623300	0. 80554100	-4. 82876900
H	4. 07553600	1. 31869700	-5. 18743000
C	0. 66347700	0. 99034700	5. 94408100
H	1. 60907300	0. 66024400	6. 36370700
C	0. 13464300	2. 26070300	6. 30920500
H	0. 66868300	2. 88175700	7. 02335800
C	-1. 03749400	2. 69756600	5. 75268600
H	-1. 45075900	3. 66834400	6. 01756300
C	0. 00223200	0. 18307700	5. 05388000
H	0. 42903100	-0. 77483500	4. 78209000
N	1. 50240100	-0. 24736800	1. 46497900
S	2. 50801400	-0. 94853400	2. 55437400
C	3. 93054300	-1. 67898900	1. 53363700

O	1. 91281100	-2. 10517300	3. 22835800
O	3. 10543000	0. 13756500	3. 33225300
F	3. 75420300	-2. 99053100	1. 38506800
F	4. 00517400	-1. 10155800	0. 33361600
F	5. 06984600	-1. 46384000	2. 19613700
H	2. 43950000	2. 55859500	2. 22047200
C	-0. 82726100	3. 41121000	1. 48690500
H	-1. 32097200	3. 83058400	0. 60705600
H	-1. 25080800	2. 43646000	1. 73846800
H	-1. 05510100	4. 08073900	2. 33123700
C	3. 42902100	3. 39154200	-0. 28695100
C	3. 79952000	2. 29150100	-1. 07200800
C	4. 24424600	3. 69612000	0. 81931800
C	4. 93152500	1. 53024700	-0. 76730600
H	3. 21196800	1. 99725900	-1. 93460100
C	5. 36715300	2. 93415900	1. 13323200
H	4. 00427400	4. 54238900	1. 45443900
C	5. 71901000	1. 84376900	0. 33675100
H	5. 17616100	0. 67633300	-1. 39037100
H	5. 96526400	3. 19373200	2. 00250700
H	6. 58864200	1. 24072600	0. 58225900
C	2. 73427000	5. 68449100	-1. 17221800
H	1. 83671900	6. 28803300	-1. 36709800
H	3. 17609700	5. 46368200	-2. 15085900
C	3. 72031100	6. 54315700	-0. 40183000
C	5. 01268000	6. 57492600	-0. 74654500
H	5. 40847000	5. 95114600	-1. 54360400
H	5. 72476600	7. 22006500	-0. 23756000
C	3. 18771000	7. 44602300	0. 68884400
H	2. 82797200	6. 88872200	1. 56388500
H	3. 95953300	8. 13742000	1. 04050900
H	2. 33712400	8. 04013900	0. 32905400

TS-1-1-5R-3

l imaginary frequency

H = -5315. 351911

G = -5315. 548632

E(M06-2X-DCM) = -5316. 234135

C	2. 18766300	4. 29315600	-0. 61469200
C	1. 26025600	4. 53242100	0. 62441600
H	1. 84915200	5. 07855700	1. 37325800
H	0. 46407400	5. 20713200	0. 29367800
C	0. 62103900	3. 37836400	1. 35860300
C	1. 30073200	3. 80595300	-1. 79834300

H	1.93371700	3.47315600	-2.62858700
H	0.73062300	4.66104700	-2.16301400
N	0.31500600	2.78259200	-1.49211600
C	-1.01341700	2.89759300	-1.84240400
N	-1.67346000	1.70636300	-1.70823100
C	-3.00239300	1.31190800	-1.92391000
C	-4.10341700	2.16694300	-2.08462900
C	-3.21626600	-0.07896500	-1.94166200
C	-5.37525700	1.62330300	-2.27147900
C	-4.49165700	-0.59834500	-2.13488700
H	-2.37626800	-0.75091500	-1.79929500
C	-5.58821700	0.24632900	-2.30943000
H	-6.57980000	-0.15749100	-2.47419000
C	-4.69690100	-2.08658500	-2.07531800
C	-6.56467100	2.54483100	-2.35210600
F	-3.62987700	-2.77129000	-2.54735700
F	-5.77804100	-2.48237900	-2.77666300
F	-4.88721500	-2.51404100	-0.79441500
F	-6.23927900	3.76595100	-2.81723800
F	-7.12978200	2.72552100	-1.12941500
F	-7.53252200	2.04496500	-3.15268900
S	-1.71467400	4.35597200	-2.32949000
H	-3.96105500	3.23741000	-2.07223400
C	1.32296600	2.42530500	2.10457200
H	-1.07705600	0.92887500	-1.40434300
H	0.77315900	2.05465100	2.97550200
H	0.65668500	1.83433700	-1.33279000
H	1.36967400	1.21699200	1.59399300
O	-0.94856400	-1.32706300	0.97223000
O	1.25883700	-2.33784400	0.00287900
P	0.51853400	-0.93887600	0.36841500
O	0.25524300	-0.05833100	-0.80961000
C	-1.23927800	-3.85817000	4.30460100
C	-0.93782300	-4.37488800	3.05023800
C	-0.94918600	-3.55122700	1.91435300
C	-1.51164200	-1.63380800	3.31781500
C	-1.57033800	-2.51037100	4.41588100
C	0.69144800	-3.12447100	-1.01899100
C	-0.35218500	-3.98542300	-0.69057600
C	-1.02174000	-4.66919900	-1.71823600
C	-0.59690400	-4.56093300	-3.03734600
C	0.50981400	-3.76549800	-3.32884600
C	1.17135700	-3.01961000	-2.33852700
H	-1.86580600	-2.10515200	5.37875400

H	0.87134600	-3.69383900	-4.35041600
C	-0.89260700	-4.42569500	0.66391800
C	-0.09875500	-5.65401800	1.21890300
H	-0.25317900	-6.55564200	0.61785800
H	0.97105600	-5.41665700	1.20403800
H	-3.09455400	-5.32560900	-1.76928400
H	-1.96817300	-6.53009200	-1.14236900
C	-1.12642900	-2.17760100	2.07618200
H	-1.24135400	-4.49606500	5.18461000
H	-1.11382800	-5.09095000	-3.83303100
C	-0.58086200	-5.79739800	2.67851300
H	-1.45367900	-6.46100400	2.75141500
H	0.18892100	-6.21630000	3.33637000
C	-2.18961700	-5.45401000	-1.16652300
C	-2.33947200	-4.87109400	0.25354000
H	-2.77559400	-5.57354800	0.96989600
H	-2.98724300	-3.98931400	0.21392500
C	2.36485100	-2.21059200	-2.74473000
C	3.66356400	-2.68486700	-2.43749500
C	2.19868400	-1.05348000	-3.54326600
C	3.89531800	-3.87232000	-1.67213000
C	4.81950400	-1.97349300	-2.93490100
C	3.36337200	-0.35375900	-4.03783000
C	5.16500800	-4.30913100	-1.39866200
H	3.04383500	-4.43269400	-1.30335000
C	6.12758400	-2.46179600	-2.62508000
C	4.63834900	-0.83258300	-3.72267000
C	6.29992900	-3.59436800	-1.87625200
H	5.31033200	-5.21172100	-0.81150700
H	6.98538200	-1.91179100	-3.00525000
H	5.51174600	-0.30976300	-4.10817900
H	7.29892700	-3.95592000	-1.64851200
C	-1.93988300	-0.21469100	3.53642500
C	-3.13792400	0.26111900	2.94132700
C	-1.23786600	0.59907000	4.46324300
C	-3.92053400	-0.51597900	2.02812900
C	-3.63370600	1.57708400	3.28446900
C	-1.76341200	1.89960800	4.81902700
C	-5.06568500	-0.01838300	1.46365000
H	-3.59967600	-1.52026800	1.77908000
C	-4.82620400	2.06339200	2.66121800
C	-2.94496300	2.34958800	4.22372600
C	-5.52039700	1.29612400	1.76613500
H	-5.62728700	-0.63464000	0.76997200

H	-5.16654300	3.06446300	2.91565100
H	-3.33796600	3.32760800	4.49563900
H	-6.40727200	1.68490700	1.27472600
C	0.78346900	0.58955400	-4.67418700
H	-0.20502300	0.96593600	-4.92230800
C	0.91182700	-0.53095800	-3.89539100
H	0.02778700	-1.03489000	-3.52444600
C	1.93522600	1.27380100	-5.16029700
H	1.81329500	2.15695500	-5.78151100
C	3.18638200	0.81261500	-4.84828700
H	4.07386700	1.32210600	-5.21666100
C	0.65267000	1.00520700	5.96098500
H	1.59905500	0.67955600	6.38235200
C	0.11651500	2.27236000	6.32650900
H	0.64583600	2.89534600	7.04246900
C	-1.05630200	2.70414100	5.76754200
H	-1.47467300	3.67278700	6.03211700
C	-0.00227000	0.19568600	5.06822000
H	0.43064100	-0.75921600	4.79539600
N	1.49737700	-0.22057000	1.47172900
S	2.51361000	-0.91467500	2.55514700
C	3.93601100	-1.63395100	1.52466700
O	1.93130700	-2.07608700	3.23218600
O	3.10767900	0.17516900	3.33054700
F	3.77996600	-2.95002500	1.39494500
F	3.98609600	-1.07118500	0.31644100
F	5.08057200	-1.39117100	2.16894500
H	2.38398700	2.58302100	2.27821400
C	-0.86898300	3.41466900	1.47029000
H	-1.34945000	3.82429200	0.57868100
H	-1.28981100	2.43850900	1.72096800
H	-1.11752000	4.08826500	2.30561000
C	3.38217600	3.38242800	-0.28382700
C	3.77962700	2.32278000	-1.11025000
C	4.16054400	3.63100200	0.86316000
C	4.90383800	1.54873400	-0.80834100
H	3.22026500	2.07127400	-2.00448900
C	5.27811900	2.85807000	1.17060600
H	3.90213300	4.45188200	1.52405200
C	5.65736700	1.80842900	0.33264000
H	5.16872500	0.72577800	-1.46400600
H	5.84801900	3.07450800	2.07012000
H	6.51928100	1.19357000	0.57560200
C	2.68887800	5.70843500	-1.11947000

H	1. 78958200	6. 31615100	-1. 27514400
H	3. 12617800	5. 54230700	-2. 11269200
C	3. 67276800	6. 51160300	-0. 28549100
C	3. 25176900	7. 34064100	0. 67921400
H	2. 19688600	7. 47289300	0. 90805600
H	3. 94886400	7. 93830000	1. 26137300
C	5. 13170900	6. 41962400	-0. 66434600
H	5. 27965200	6. 80110400	-1. 68451400
H	5. 76131100	7. 00900100	0. 00958000
H	5. 49107300	5. 38537700	-0. 65758000

TS-1-1-5R-4

l imaginary frequency

H = -5315. 341365

G = -5315. 538530

E(M06-2X-DCM) = -5316. 225332

C	-2. 23387400	4. 64756200	-0. 05371800
C	-1. 96058800	4. 30043600	1. 45950500
H	-2. 92817500	4. 16522100	1. 94602700
H	-1. 52571800	5. 21629200	1. 88802000
C	-1. 02341800	3. 21874700	1. 91074400
C	-0. 92845900	4. 77828000	-0. 87701400
H	-1. 15309700	5. 26621700	-1. 83400900
H	-0. 22921300	5. 44766600	-0. 36872600
N	-0. 25658200	3. 51004100	-1. 10150900
C	1. 02341400	3. 43550400	-1. 59318500
N	1. 45801500	2. 13964600	-1. 68510900
C	2. 66915700	1. 57797400	-2. 12252100
C	3. 84876800	2. 28053200	-2. 39536200
C	2. 67165100	0. 17360300	-2. 24324800
C	5. 00506800	1. 57867800	-2. 75172300
C	3. 82950800	-0. 50047400	-2. 60869500
H	1. 76318700	-0. 38042200	-2. 04006400
C	5. 01707900	0. 19310500	-2. 86344600
H	5. 92344900	-0. 33477400	-3. 13486800
C	3. 81295600	-1. 99461600	-2. 77411900
C	6. 27981400	2. 36368900	-2. 91111500
F	2. 68485200	-2. 55497200	-2. 27858000
F	3. 88854700	-2. 35615800	-4. 07957100
F	4. 85955100	-2. 58640500	-2. 15211800
F	7. 25058700	1. 64851700	-3. 51898800
F	6. 09478400	3. 49174000	-3. 62633400
F	6. 76747500	2. 74456000	-1. 70130600
S	1. 88993700	4. 82756000	-1. 98090800

C	-2.84081800	6.10538200	-0.04728200
H	-3.12335700	6.34433600	-1.07937900
H	-2.02576900	6.78970100	0.21965200
H	3.86438100	3.35814500	-2.31488500
C	-1.49139100	2.08039200	2.58981500
H	0.88672400	1.45349200	-1.18050600
H	-2.51028600	2.11910900	2.97978600
H	-0.77148200	1.61558300	3.26729500
H	-0.84726100	2.68823200	-1.17986700
H	-1.61273300	1.11150400	1.79476100
O	0.27900300	-1.70364200	1.86430900
O	-0.47609400	-1.83693900	-0.63636600
P	-0.36778500	-0.83968500	0.64325300
O	0.44459300	0.33459000	0.21226100
C	4.22364700	-3.05432100	1.41963900
C	3.16188700	-3.76657200	0.87380700
C	1.83825900	-3.35483800	1.09064900
C	2.64638000	-1.44802900	2.38528800
C	3.95440500	-1.93069500	2.19758500
C	-1.07330100	-3.10732200	-0.68884200
C	-0.52615900	-4.17058200	0.03172800
C	-1.27184300	-5.35350400	0.16392700
C	-2.44061100	-5.53983200	-0.56307300
C	-2.84743900	-4.54231900	-1.44428200
C	-2.19531200	-3.29773600	-1.52283400
H	4.77154100	-1.39153900	2.66688600
H	-3.70848500	-4.70911100	-2.08294400
C	0.87168600	-4.42083400	0.59830600
C	1.75585600	-5.12042900	-0.49582000
H	1.43898400	-6.14992000	-0.68440300
H	1.66122100	-4.56781900	-1.43434400
H	-0.20379600	-7.19301100	0.60605200
H	-1.29412200	-6.68117400	1.88844900
C	1.60052300	-2.16604900	1.77260300
H	5.24965600	-3.37428300	1.25841800
H	-3.00902400	-6.46265500	-0.48047600
C	3.20551200	-5.01212900	0.02054700
H	3.93416100	-4.92337200	-0.79268600
H	3.49284700	-5.89046300	0.61511300
C	-0.59972000	-6.30995500	1.12586800
C	0.53291800	-5.44847100	1.72598600
H	0.16220200	-4.90203900	2.60110300
H	1.40712200	-6.03016400	2.03519800
C	-2.68468800	-2.32640100	-2.55207800

C	-4.06024800	-1.97011600	-2.58055900
C	-1.82977800	-1.92212600	-3.61424000
C	-4.97021500	-2.28825500	-1.51845600
C	-4.59552800	-1.26363900	-3.72229400
C	-2.36942100	-1.14373200	-4.70793300
C	-6.30781100	-1.99888600	-1.61279500
H	-4.58370900	-2.74261700	-0.61510300
C	-6.00102200	-1.00393500	-3.79221000
C	-3.73545200	-0.85494100	-4.74278300
C	-6.84023900	-1.37066900	-2.77459200
H	-6.96953200	-2.24851800	-0.78782900
H	-6.38641100	-0.50500900	-4.67889000
H	-4.14033100	-0.31070400	-5.59387100
H	-7.90675200	-1.17216000	-2.84132900
C	2.45577100	-0.25574600	3.26863200
C	3.07935400	0.97394700	2.93365800
C	1.78029900	-0.39505800	4.50915100
C	3.75683800	1.19129800	1.68838100
C	3.04630600	2.07240000	3.87433700
C	1.70988900	0.73068000	5.41498100
C	4.39340900	2.37501300	1.41506700
H	3.75429000	0.40105600	0.94736000
C	3.72400400	3.29098400	3.55135900
C	2.35091500	1.92669400	5.07802600
C	4.38636700	3.43837600	2.36263100
H	4.90932100	2.50710300	0.46852100
H	3.70254200	4.09922100	4.27915500
H	2.32515400	2.75777900	5.78057400
H	4.90049100	4.36684200	2.13068500
C	0.34803100	-1.86955900	-4.73566200
H	1.39360300	-2.16043800	-4.76188000
C	-0.44613100	-2.28435900	-3.69738000
H	-0.01444900	-2.90690500	-2.92460500
C	-0.18267500	-1.06463700	-5.78230500
H	0.46298600	-0.73914200	-6.59327800
C	-1.50640700	-0.72112100	-5.76739000
H	-1.93506300	-0.12471400	-6.56947400
C	0.54544400	-1.72526400	6.14810300
H	0.10522300	-2.67290400	6.44601500
C	0.44651200	-0.60260900	7.01736100
H	-0.07247200	-0.69978700	7.96697300
C	1.01816300	0.58777400	6.65897100
H	0.96881800	1.44919700	7.32103200
C	1.18987700	-1.62539300	4.94296400

H	1.26068400	-2.49630300	4.30290900
N	-1.79920900	-0.31640400	1.26883500
S	-3.05134700	-1.09226800	1.95047900
C	-2.52371700	-1.51343300	3.70556200
O	-4.11410300	-0.09894400	2.14019500
O	-3.33711600	-2.39356100	1.34293600
F	-3.61550900	-1.81339600	4.41377500
F	-1.91586600	-0.46194100	4.27429800
F	-1.69773700	-2.56077200	3.72106400
C	-3.20136500	3.66891500	-0.74222400
C	-3.79211900	2.57522300	-0.09660200
C	-3.55348800	3.89923800	-2.08642300
C	-4.72056600	1.75983400	-0.74997200
H	-3.55950400	2.33612300	0.93231800
C	-4.48158400	3.09262800	-2.73863700
H	-3.10845500	4.72479100	-2.63458300
C	-5.07937200	2.02330600	-2.06903500
H	-5.14848600	0.91850600	-0.21466500
H	-4.73754400	3.30236900	-3.77394000
H	-5.80304300	1.39198800	-2.57252400
C	-4.02080000	6.38872000	0.86344300
C	-3.86019300	7.13932900	1.96098300
H	-4.69499100	7.38222900	2.61369400
H	-2.89358200	7.55248400	2.24068300
C	-5.38033700	5.86691000	0.46190700
H	-6.15661500	6.22902000	1.14288100
H	-5.63679800	6.19295100	-0.55462900
H	-5.41624300	4.77236800	0.45093000
C	0.44955700	3.42847100	1.82204600
H	0.94440600	2.51707800	1.46981900
H	0.74618900	4.27353000	1.20347800
H	0.82184600	3.59462600	2.84337400

TS-1-1-5R-5

l imaginary frequency

H = -5315.338726

G = -5315.535849

E(M06-2X-DCM) = -5316.224476

C	-2.03466300	4.70480600	-0.33077400
C	-1.76517800	4.48042600	1.20667700
H	-2.73668900	4.45851800	1.70467000
H	-1.24719700	5.39162400	1.53876100
C	-0.91097500	3.36433200	1.73446400
C	-0.71833900	4.75314100	-1.14331400

H	-0.91161600	5.19423700	-2.12941700
H	-0.00721600	5.42981100	-0.66148200
N	-0.08362300	3.45416000	-1.28469600
C	1.19933400	3.30585800	-1.74904800
N	1.58106700	1.99020700	-1.77049600
C	2.76961100	1.35594500	-2.16627600
C	3.97829900	1.99273600	-2.47133400
C	2.71364200	-0.05208200	-2.20940000
C	5.10520700	1.22453000	-2.78236000
C	3.84274600	-0.79279500	-2.53282700
H	1.78200000	-0.55588500	-1.98126500
C	5.05923300	-0.16433100	-2.81882600
H	5.94323700	-0.74362200	-3.05716600
C	3.76400000	-2.29172300	-2.61824600
C	6.41187500	1.94629900	-2.97840000
F	2.60359200	-2.77618200	-2.11731900
F	3.84790400	-2.72570100	-3.90078300
F	4.77208300	-2.89306100	-1.94392400
F	7.35648000	1.15677300	-3.53311400
F	6.27715900	3.03479300	-3.76296700
F	6.90671300	2.38089000	-1.79003000
S	2.12773700	4.64179200	-2.18796400
C	-2.64264100	6.15612200	-0.45899800
H	-2.90807000	6.29370500	-1.51160300
H	-1.83540500	6.87065800	-0.24756000
H	4.03846400	3.07166000	-2.45057800
C	-1.45938300	2.28789900	2.45443300
H	0.97183400	1.35444100	-1.24463800
H	-2.48035700	2.40313100	2.82240900
H	-0.77923600	1.81807700	3.16870700
H	-0.70051100	2.64883800	-1.32038400
H	-1.61549000	1.29293100	1.70758400
O	0.17670700	-1.58970300	1.94629000
O	-0.56349200	-1.82851300	-0.55181700
P	-0.43334500	-0.76993300	0.67603000
O	0.42406800	0.35102700	0.19215700
C	4.06187200	-3.13266900	1.61048300
C	2.97316400	-3.82720300	1.09599200
C	1.66755400	-3.34637500	1.27728400
C	2.55019800	-1.40902000	2.47353000
C	3.83704300	-1.95739500	2.32328300
C	-1.21438700	-3.07329500	-0.54453900
C	-0.72207900	-4.11693100	0.24124100
C	-1.51953700	-5.25747500	0.42995900

C	-2.68717400	-5.43432000	-0.30122600
C	-3.03936900	-4.47236000	-1.24331400
C	-2.33288200	-3.26309700	-1.38335200
H	4.67387300	-1.42974000	2.77041800
H	-3.89878800	-4.63890400	-1.88415200
C	0.65842500	-4.39515500	0.83601300
C	1.51879400	-5.19308800	-0.20870300
H	1.15746300	-6.21633000	-0.34351900
H	1.45617200	-4.68961500	-1.17721100
H	-0.53712500	-7.11334600	0.98707000
H	-1.61575700	-6.48317200	2.22609400
C	1.47741500	-2.11217700	1.89036100
H	5.07378100	-3.50552600	1.47616500
H	-3.29637800	-6.32561200	-0.17478400
C	2.96761000	-5.12021500	0.31547800
H	3.70613600	-5.11090800	-0.49357800
H	3.21010500	-5.97480700	0.96235400
C	-0.89886600	-6.18606800	1.45193800
C	0.26504400	-5.34176400	2.01575000
H	-0.08943600	-4.73093800	2.85423700
H	1.10996700	-5.94236200	2.36732400
C	-2.76530400	-2.33615700	-2.47710600
C	-4.12571900	-1.93169600	-2.55383600
C	-1.87794400	-2.03055100	-3.54576000
C	-5.06348500	-2.14592600	-1.48998300
C	-4.61603100	-1.28371100	-3.74921900
C	-2.37010300	-1.30441400	-4.69642900
C	-6.38862200	-1.81996100	-1.62963100
H	-4.70779500	-2.55055700	-0.55078700
C	-6.01036900	-0.98285800	-3.86377800
C	-3.72422900	-0.97178100	-4.77672800
C	-6.87922800	-1.25465600	-2.84111700
H	-7.07258000	-1.99096800	-0.80274800
H	-6.36293200	-0.52996600	-4.78798300
H	-4.09483500	-0.47146200	-5.66942600
H	-7.93709100	-1.02633300	-2.94181800
C	2.40830200	-0.16682600	3.29514600
C	3.08970200	1.01528300	2.90593600
C	1.72192600	-0.21515400	4.53664600
C	3.78287500	1.14063400	1.65661600
C	3.10237200	2.15854400	3.79219200
C	1.69920400	0.95509400	5.38679700
C	4.47379200	2.27970800	1.33067500
H	3.74843400	0.31588400	0.95497400

C	3. 83605500	3. 32818400	3. 41511500
C	2. 39552500	2. 10311600	4. 99676200
C	4. 51005700	3. 38743400	2. 22528600
H	4. 99968000	2. 34215000	0. 38246900
H	3. 84760500	4. 17119600	4. 10257700
H	2. 40484300	2. 96751400	5. 65835400
H	5. 06655700	4. 27949000	1. 95196100
C	0. 31909100	-2. 12642500	-4. 62650000
H	1. 35345300	-2. 45587800	-4. 61464000
C	-0. 50736000	-2. 44659700	-3. 57997000
H	-0. 11174600	-3. 03435600	-2. 76206000
C	-0. 16385400	-1. 37069500	-5. 73129600
H	0. 50692200	-1. 12013100	-6. 54848400
C	-1. 47425100	-0. 98041900	-5. 76338500
H	-1. 86719900	-0. 42135400	-6. 60947300
C	0. 42262600	-1. 40768400	6. 23084000
H	-0. 06090300	-2. 31909800	6. 57157000
C	0. 37129900	-0. 24096800	7. 04436600
H	-0. 15482200	-0. 26869200	7. 99462100
C	0. 99715300	0. 90386700	6. 63214400
H	0. 98450100	1. 79768500	7. 25162800
C	1. 07489400	-1. 39523000	5. 02585500
H	1. 10822300	-2. 29837900	4. 42896600
N	-1. 84926700	-0. 16747600	1. 26048500
S	-3. 13084000	-0. 85824900	1. 97721200
C	-2. 61501600	-1. 22638600	3. 74768000
O	-4. 14877000	0. 18642500	2. 13098200
O	-3. 47665900	-2. 16985300	1. 42525200
F	-3. 71600900	-1. 44595900	4. 47111900
F	-1. 95933800	-0. 17819100	4. 26777100
F	-1. 83592600	-2. 30778000	3. 80989800
C	-3. 01977000	3. 69029900	-0. 93413600
C	-3. 75618200	2. 77611500	-0. 17185100
C	-3. 26153200	3. 72414800	-2. 32183900
C	-4. 70598400	1. 93680500	-0. 75959300
H	-3. 61868200	2. 69830100	0. 89803200
C	-4. 21427500	2. 89684600	-2. 90965700
H	-2. 71148600	4. 41319400	-2. 95636100
C	-4. 94849500	2. 00217100	-2. 12829500
H	-5. 24022200	1. 22956100	-0. 13391300
H	-4. 37962400	2. 95016100	-3. 98248400
H	-5. 68793700	1. 35261100	-2. 58314400
C	-3. 84636500	6. 49391600	0. 41062500
C	-5. 07913400	6. 07639000	0. 10065400

H	-5.93418400	6.33106300	0.72224900
H	-5.28170900	5.47101200	-0.77741000
C	-3.59528700	7.38016300	1.60972200
H	-4.51747000	7.57194500	2.16663600
H	-2.86738000	6.94338700	2.30635000
H	-3.18116900	8.34895300	1.29758400
C	0.57244200	3.47921100	1.66120400
H	1.01575300	2.52191100	1.36679900
H	0.92802100	4.27086700	1.00382200
H	0.93958400	3.67786300	2.67882700

TS-1-2-5S

l imaginary frequency

H = -5315.346483

G = -5315.547863

E(M06-2X-DCM) = -5316.237966

O	-2.02000900	0.01809200	1.96103400
O	-3.02165300	-1.43756000	0.05632200
P	-1.86012300	-0.34954100	0.39173400
O	-2.07521600	0.97965400	-0.31926400
N	-0.43858100	-1.08725100	0.20873800
S	0.01458400	-1.93479900	-1.06257700
C	-0.26825200	-3.72064400	-0.57573600
F	0.09369300	-4.50973300	-1.58886300
F	0.46885800	-4.02640900	0.49888200
F	-1.55567900	-3.93000000	-0.29119500
C	0.61801700	3.93984400	-0.92532200
C	0.86712600	3.33743600	-2.35057200
H	0.55048800	4.07841400	-3.09823300
H	1.94806800	3.23039500	-2.47144900
C	0.20338300	2.05023300	-2.75609700
C	1.01216400	2.86006700	0.15666600
H	0.10336800	2.46066900	0.60369500
H	1.59262100	3.33155800	0.95136800
N	1.71475900	1.66520800	-0.32714300
C	3.07962400	1.51910200	-0.42874800
N	3.43063400	0.23872700	-0.76702600
C	4.69237200	-0.37677300	-0.90204600
C	5.87678000	0.28337300	-1.25879100
C	4.71837700	-1.76719500	-0.71311900
C	7.06150200	-0.44461400	-1.38118800
C	5.91233600	-2.47319800	-0.83221200
H	3.80092200	-2.29070800	-0.46772300
C	7.09959600	-1.82098600	-1.16158000

H	8.02621300	-2.37264100	-1.25830900
C	5.90455100	-3.94464200	-0.51893000
C	8.33626200	0.28968200	-1.70757500
F	5.79849200	-4.16093400	0.82077100
F	7.03157800	-4.56298800	-0.92728500
F	4.85890200	-4.57784800	-1.09106600
F	9.22889400	-0.50990300	-2.33451100
F	8.94324100	0.75507000	-0.59154300
F	8.11469800	1.35499900	-2.50777900
S	4.15636800	2.79136200	-0.19451200
C	1.57460000	5.20004500	-0.85855700
H	2.59471600	4.82991800	-0.98091700
H	1.34037400	5.82198400	-1.73318300
H	5.87289100	1.34835900	-1.43601300
C	-1.16609200	1.81749700	-2.62875500
H	2.66449200	-0.43880000	-0.81923400
H	-1.81764000	2.68327900	-2.51666100
H	-1.57065100	1.00203200	-3.22958500
O	1.48582700	-1.84833400	-1.18954600
H	1.19346300	0.80250400	-0.18123300
O	-0.78001000	-1.71864600	-2.28256000
H	-1.41742800	1.33737800	-1.46045300
C	-7.00076700	-0.17691700	0.45167300
C	-6.26954700	-0.57585000	1.56507300
C	-4.96893300	-1.08367500	1.42141400
C	-5.09497800	-0.71405300	-0.99002100
C	-6.42275400	-0.28637600	-0.81209300
C	-1.93898700	-0.97551200	2.94885400
C	-3.04650500	-1.78612600	3.19391200
C	-2.91423200	-2.86765000	4.08021700
C	-1.73973100	-3.05786700	4.79895300
C	-0.69019000	-2.15754700	4.62918100
C	-0.75165800	-1.10905400	3.69418100
H	-6.99631500	-0.01554800	-1.69332400
H	0.21719600	-2.26935600	5.21436500
C	-4.50143900	-1.67528700	2.74598100
C	-5.33265500	-0.80189300	3.74600000
H	-5.44720400	-1.28064500	4.72311900
H	-4.81089100	0.14979000	3.89966600
H	-3.96480300	-4.77738700	4.03370600
H	-4.74363100	-3.54945100	5.02539100
C	-4.37113300	-1.06960600	0.16368800
H	-8.01369300	0.20317800	0.55758800
H	-1.64109400	-3.88713500	5.49477400

C	-6.67379700	-0.55176900	3.02295800
H	-7.40425400	-1.34146900	3.24733300
H	-7.13967300	0.39713500	3.31231700
C	-4.17475100	-3.70369900	4.09786500
C	-4.94303400	-3.17297500	2.86974700
H	-6.02858700	-3.28286100	2.95218900
H	-4.61961200	-3.70947200	1.97026900
C	0.41233500	-0.17728600	3.58576700
C	0.26580700	1.18527100	3.95320300
C	1.68979200	-0.68814500	3.24170300
C	-0.98153300	1.75711800	4.36507700
C	1.42377800	2.05143100	3.95354200
C	2.84513400	0.17911400	3.29985300
C	-1.08658200	3.08129000	4.70473700
H	-1.85874000	1.12327000	4.41828400
C	1.27007300	3.42937300	4.30650100
C	2.67931100	1.52468800	3.63763000
C	0.05093900	3.93705000	4.66584500
H	-2.04737800	3.48269800	5.01661700
H	2.15187200	4.06468500	4.28680700
H	3.54984400	2.17618600	3.65899100
H	-0.05185800	4.98509500	4.93315000
C	-4.54405200	-0.80689500	-2.37671200
C	-4.20819500	-2.07080300	-2.92395600
C	-4.45881100	0.36064100	-3.17635900
C	-4.31552600	-3.29382300	-2.18807100
C	-3.76400500	-2.15797700	-4.29646200
C	-4.05092300	0.25084700	-4.55967900
C	-3.97525500	-4.49731900	-2.74743700
H	-4.67884400	-3.26378300	-1.16767400
C	-3.41469500	-3.43269600	-4.84144300
C	-3.70684000	-1.00077200	-5.07700500
C	-3.51016200	-4.57206000	-4.09059200
H	-4.06324000	-5.40805100	-2.16126500
H	-3.07228800	-3.47396000	-5.87265100
H	-3.39253400	-1.07744000	-6.11604200
H	-3.23995400	-5.53512300	-4.51474000
C	3.15969900	-2.51633200	2.55339200
H	3.29444700	-3.54418400	2.22787100
C	1.90188900	-2.04254700	2.82291100
H	1.04550500	-2.69251400	2.69552500
C	4.30016800	-1.67097600	2.66936700
H	5.28454000	-2.07266600	2.45146800
C	4.14067400	-0.35676600	3.01509700

H	4.99627500	0.31108100	3.07376800
C	-4.68415700	2.77768600	-3.48497800
H	-4.89901300	3.75896400	-3.07125400
C	-4.32140700	2.65647900	-4.85709700
H	-4.28727200	3.54169500	-5.48667700
C	-4.00477900	1.42823700	-5.37162400
H	-3.71116700	1.32149400	-6.41346000
C	-4.74504000	1.67292500	-2.67469300
H	-4.99404200	1.79020000	-1.62673300
C	-0.82556200	4.45139900	-0.72782800
C	-1.47222500	5.16661700	-1.75242700
C	-1.49944900	4.34611800	0.49885700
C	-2.73761200	5.72431000	-1.57419700
H	-0.98438900	5.30894600	-2.71283000
C	-2.76651900	4.90505600	0.68320700
H	-1.04263400	3.84662100	1.34485300
C	-3.39690700	5.59360500	-0.35068800
H	-3.20249600	6.26895000	-2.39211800
H	-3.25543600	4.79799000	1.64762200
H	-4.38215700	6.02831200	-0.20577700
C	1.51576900	6.07583000	0.38430900
C	2.33591300	5.85732800	1.42060000
H	3.06049700	5.04822500	1.41868300
H	2.31903700	6.50196100	2.29679800
C	0.57912300	7.26259900	0.37147200
H	-0.46975500	6.96693800	0.26799000
H	0.67840500	7.85282500	1.28820500
H	0.80636900	7.92140100	-0.47866900
C	1.04998300	1.03973800	-3.45972500
H	2.05473800	0.96536800	-3.03799200
H	0.57539800	0.05599200	-3.49146400
H	1.16585800	1.39071700	-4.49859800

TS-1-2-5S-1

l imaginary frequency

H = -5315.346397

G = -5315.547638

E(M06-2X-DCM) = -5316.237871

O	-2.02245900	0.02528200	1.95903700
O	-3.01782800	-1.44173200	0.05975900
P	-1.85928400	-0.34947200	0.39175000
O	-2.07622100	0.97565000	-0.32630400
N	-0.43569800	-1.08472700	0.21506500
S	0.02326100	-1.93159500	-1.05456900

C	-0.25160500	-3.71791500	-0.56516400
F	0.11281700	-4.50686300	-1.57748400
F	0.48751700	-4.01929300	0.50933700
F	-1.53799200	-3.93185400	-0.27944300
C	0.60875300	3.94116400	-0.93578000
C	0.86571900	3.33343200	-2.35729200
H	0.54931300	4.06987600	-3.10952400
H	1.94753400	3.22990200	-2.47336600
C	0.20843500	2.04192200	-2.75974800
C	1.00395900	2.86811100	0.15250300
H	0.09529500	2.46689800	0.59819800
H	1.57945000	3.34593000	0.94704500
N	1.71347700	1.67369300	-0.32265800
C	3.07959900	1.53262000	-0.41688800
N	3.43746900	0.25060900	-0.74101200
C	4.69946900	-0.36532700	-0.87120100
C	5.89306300	0.29592100	-1.19430000
C	4.71799800	-1.75876200	-0.70137400
C	7.07705200	-0.43493700	-1.30668200
C	5.91203300	-2.46651000	-0.80572800
H	3.79568900	-2.28260900	-0.47583600
C	7.10729100	-1.81410800	-1.10452400
H	8.03646100	-2.36523000	-1.17751200
C	5.89821400	-3.93864800	-0.49619500
C	8.33763500	0.27814100	-1.72308600
F	5.80003000	-4.15821600	0.84366300
F	7.01957700	-4.56166000	-0.91326800
F	4.84573800	-4.56464900	-1.06340200
F	9.44326200	-0.33998600	-1.24934400
F	8.36701400	1.55446500	-1.28714100
F	8.46061500	0.31983500	-3.07152500
S	4.14833800	2.81306200	-0.19034500
C	1.55900700	5.20627600	-0.87134200
H	2.58128400	4.84061700	-0.98873600
H	1.32463300	5.82323400	-1.74943800
H	5.89914700	1.36599100	-1.33792900
C	-1.16056900	1.80440400	-2.63657500
H	2.67258700	-0.42801100	-0.79588200
H	-1.81589300	2.66818900	-2.53120800
H	-1.55965200	0.98430400	-3.23472100
O	1.49416900	-1.83744000	-1.18028300
H	1.19508600	0.80973700	-0.17401500
O	-0.77100700	-1.72160600	-2.27582300
H	-1.41512000	1.32961000	-1.46652600

C	-6.99927300	-0.18293500	0.43719100
C	-6.27053500	-0.57440000	1.55486500
C	-4.96916200	-1.08199500	1.41751300
C	-5.08931800	-0.72702100	-0.99641600
C	-6.41797300	-0.29962100	-0.82443300
C	-1.94293100	-0.96372900	2.95162100
C	-3.05073400	-1.77344900	3.19853500
C	-2.91993600	-2.85043400	4.09057600
C	-1.74667500	-3.03704200	4.81226400
C	-0.69685200	-2.13761700	4.63971500
C	-0.75687000	-1.09363200	3.69958800
H	-6.98958200	-0.03474000	-1.70873400
H	0.20964000	-2.24657900	5.22682100
C	-4.50468600	-1.66559400	2.74666000
C	-5.33883800	-0.78685400	3.73948000
H	-5.45558300	-1.25996200	4.71909200
H	-4.81801100	0.16602000	3.88888500
H	-3.97016900	-4.76054900	4.05256500
H	-4.75110900	-3.52717200	5.03581900
C	-4.36812900	-1.07489700	0.16128900
H	-8.01280200	0.19689200	0.53820000
H	-1.64921100	-3.86285100	5.51235100
C	-6.67834900	-0.54178700	3.01161100
H	-7.40896900	-1.33047800	3.23897100
H	-7.14539800	0.40860700	3.29411400
C	-4.18035500	-3.68654500	4.11031000
C	-4.94616600	-3.16272000	2.87774800
H	-6.03186300	-3.27238800	2.95850600
H	-4.62078100	-3.70408000	1.98190100
C	0.40754300	-0.16259400	3.58909300
C	0.26115700	1.20128800	3.95152100
C	1.68524300	-0.67531900	3.24879500
C	-0.98672400	1.77539200	4.35858100
C	1.41974600	2.06663500	3.95142200
C	2.84107400	0.19129200	3.30640000
C	-1.09157300	3.10079200	4.69350900
H	-1.86451300	1.14234300	4.41180900
C	1.26626000	3.44582400	4.29954700
C	2.67556500	1.53799200	3.63982800
C	0.04668700	3.95556100	4.65444100
H	-2.05279500	3.50398800	5.00174100
H	2.14857000	4.08043100	4.27977600
H	3.54647900	2.18899800	3.66089900
H	-0.05596000	5.00456500	4.91799200

C	-4.53448700	-0.82763000	-2.38099100
C	-4.19517900	-2.09442000	-2.91939300
C	-4.44857100	0.33504100	-3.18763000
C	-4.30323200	-3.31306000	-2.17637600
C	-3.74643600	-2.18942100	-4.28988800
C	-4.03612400	0.21726600	-4.56894300
C	-3.95942900	-4.51949100	-2.72720800
H	-4.67003100	-3.27729700	-1.15740500
C	-3.39348400	-3.46695300	-4.82585600
C	-3.68843000	-1.03698600	-5.07737500
C	-3.48976200	-4.60182100	-4.06832400
H	-4.04813600	-5.42673700	-2.13575800
H	-3.04761600	-3.51405300	-5.85565600
H	-3.37059100	-1.11959500	-6.11487700
H	-3.21676800	-5.56707700	-4.48564700
C	3.15477600	-2.50635500	2.56720400
H	3.28920500	-3.53497000	2.24400800
C	1.89699500	-2.03100900	2.83406200
H	1.04030000	-2.68067100	2.70729600
C	4.29569200	-1.66160400	2.68299900
H	5.28007400	-2.06469400	2.46770000
C	4.13666200	-0.34646400	3.02542200
H	4.99267700	0.32087300	3.08413400
C	-4.67713100	2.74969500	-3.51223300
H	-4.89507800	3.73316200	-3.10538400
C	-4.30976900	2.62050400	-4.88238900
H	-4.27515200	3.50179200	-5.51742700
C	-3.98932300	1.38960400	-5.38812100
H	-3.69215200	1.27680600	-6.42830700
C	-4.73859700	1.64997400	-2.69515500
H	-4.99106100	1.77347600	-1.64874100
C	-0.83781800	4.44715300	-0.74572200
C	-1.48363600	5.15528200	-1.77577100
C	-1.51580900	4.34436500	0.47890100
C	-2.75193100	5.70854800	-1.60461200
H	-0.99281700	5.29548000	-2.73496800
C	-2.78583400	4.89888800	0.65617200
H	-1.06013100	3.85030000	1.32869400
C	-3.41520200	5.58041300	-0.38297600
H	-3.21599400	6.24778700	-2.42656900
H	-3.27791100	4.79398800	1.61921900
H	-4.40273700	6.01171500	-0.24355300
C	1.49169200	6.08716500	0.36749200
C	2.30870800	5.87674700	1.40791800

H	3.03685400	5.07086600	1.41239100
H	2.28556500	6.52505400	2.28125400
C	1.06186500	1.03199600	-3.45587600
H	2.06483200	0.96263900	-3.02907400
H	0.59096700	0.04651100	-3.48664200
H	1.18164600	1.38006200	-4.49529100
C	0.55003500	7.26984000	0.34588500
H	0.77793900	7.92603300	-0.50609700
H	-0.49713900	6.96926600	0.23936900
H	0.64306300	7.86433200	1.26051400

TS-1-2-5S-2

l imaginary frequency

H = -5315.344363

G = -5315.545578

E(M06-2X-DCM) = -5316.234277

O	-1.58798800	-1.85277100	-1.31729900
O	-3.19990000	-0.34031000	0.04720300
P	-1.65082400	-0.78536800	-0.10575800
O	-0.93536900	0.54042400	-0.45669000
N	-1.20485800	-1.53528500	1.22844400
S	0.33681000	-1.74496600	1.60434500
C	0.47026200	-3.60405400	1.72418000
F	0.10501700	-4.16403000	0.57036800
F	-0.31601000	-4.06527800	2.70320900
F	1.73787300	-3.92673700	1.99150700
C	-0.12085300	4.45312200	-0.41855500
C	0.06276500	4.25220300	1.13514400
H	-0.71725200	4.83539200	1.64003100
H	1.02071400	4.71109500	1.39753500
C	-0.00001200	2.87744500	1.75659200
C	1.03530700	3.71170900	-1.15569200
H	0.74443200	3.52777100	-2.19464300
H	1.92535700	4.33632300	-1.15380600
N	1.47365400	2.44971000	-0.55816400
C	2.79293600	2.23214700	-0.20142400
N	3.04464100	0.93084500	0.13340700
C	4.24676600	0.28892500	0.51918800
C	5.32583000	0.91847600	1.15599500
C	4.31315200	-1.09297600	0.28282000
C	6.44992200	0.17239300	1.51386600
C	5.44116300	-1.82065600	0.65404600
H	3.47274300	-1.60011400	-0.17366000
C	6.52713300	-1.19689800	1.26561600

H	7.40653800	-1.76273000	1.54680500
C	5.48767700	-3.28933100	0.33076100
C	7.57114700	0.85281300	2.25585900
F	5.77230500	-3.50235500	-0.98710800
F	6.43383600	-3.94030000	1.03784500
F	4.30649800	-3.89735600	0.56668000
F	8.75924300	0.24511000	2.03470800
F	7.70417900	2.14720100	1.89943800
F	7.36525900	0.83246000	3.59440700
S	3.92832700	3.48085700	-0.13601200
H	5.29511900	1.97840300	1.35662400
C	-1.12333700	2.06197000	1.69963100
H	2.26403100	0.27291600	0.07556800
H	-2.07977000	2.50021500	1.42021500
H	-1.18213700	1.25262800	2.42931000
O	1.25938200	-1.38707600	0.49787600
H	0.92803400	1.62727700	-0.80880400
O	0.64646900	-1.23020600	2.94169100
H	-0.92345800	1.31514400	0.58277000
C	-6.01130700	-3.28429200	1.02259400
C	-5.59045200	-3.11749500	-0.29234900
C	-4.71152500	-2.07807900	-0.63692600
C	-4.61976900	-1.39246300	1.70969600
C	-5.55161600	-2.40273900	2.00089700
C	-1.99735200	-1.54578000	-2.62348600
C	-3.35829200	-1.48594400	-2.91515200
C	-3.75614500	-1.01065700	-4.17548100
C	-2.81346700	-0.74747500	-5.16399500
C	-1.46331600	-0.97120100	-4.89298500
C	-1.01614200	-1.35841300	-3.61767000
H	-5.89983800	-2.50092700	3.02469600
H	-0.72502100	-0.83230500	-5.67676700
C	-4.58555700	-1.98761300	-2.15506000
C	-4.89025100	-3.47711500	-2.54054300
H	-3.97263600	-4.06499700	-2.42288400
H	-5.22098600	-3.58017600	-3.57825000
H	-5.70449600	-1.64961900	-4.88511600
H	-5.57590100	0.09004900	-4.65479800
C	-4.18244900	-1.28484500	0.37661400
H	-6.69703700	-4.08454700	1.28886700
H	-3.12154300	-0.39887500	-6.14649600
C	-5.94118000	-3.94248300	-1.51060200
H	-5.89353200	-5.01972600	-1.31556500
H	-6.96269700	-3.72969500	-1.85559600

C	-5.26239400	-0.87581200	-4.24250500
C	-5.68477100	-1.05667100	-2.76753400
H	-5.65647300	-0.09031500	-2.25098900
H	-6.69201100	-1.46816800	-2.65146800
C	0.43543600	-1.62348800	-3.37390300
C	1.39483200	-0.59631400	-3.56326600
C	0.85590100	-2.93260800	-3.02105700
C	1.04944200	0.74207800	-3.94228900
C	2.79848900	-0.88646600	-3.36905400
C	2.25805300	-3.19363300	-2.78906900
C	2.01015000	1.69934400	-4.14904700
H	0.00587400	0.99955100	-4.07420000
C	3.76636900	0.14529000	-3.58013400
C	3.18925400	-2.16755700	-2.97096800
C	3.39051500	1.40292200	-3.96703600
H	1.71316600	2.70030900	-4.45100500
H	4.81466800	-0.09593900	-3.42325400
H	4.24220300	-2.37146200	-2.79372000
H	4.13540700	2.17765600	-4.12223900
C	-4.17899600	-0.46355700	2.79713800
C	-3.44233500	-0.96078100	3.90028400
C	-4.57909300	0.89649500	2.76075100
C	-2.97544000	-2.31254700	3.97839200
C	-3.11731800	-0.07691200	4.99783500
C	-4.22373400	1.77377900	3.85388900
C	-2.27449000	-2.76166100	5.06616100
H	-3.15554500	-2.97775100	3.14310600
C	-2.39179000	-0.58942900	6.11874400
C	-3.51198100	1.26218600	4.94263000
C	-1.98627600	-1.89499600	6.15828500
H	-1.91531700	-3.78635900	5.08863500
H	-2.16435500	0.08882300	6.93776200
H	-3.26106600	1.92328600	5.76997600
H	-1.42985600	-2.27198800	7.01187500
C	0.39881700	-5.28846200	-2.55200000
H	-0.30926000	-6.10975600	-2.47893500
C	-0.04299800	-4.04160900	-2.90935300
H	-1.09428800	-3.89225000	-3.12654000
C	1.77431500	-5.52381400	-2.27304900
H	2.10210800	-6.51522600	-1.97302600
C	2.67720800	-4.50343500	-2.39460600
H	3.73104700	-4.66292400	-2.18718200
C	-5.70851900	2.78013300	1.68131000
H	-6.29288400	3.17453400	0.85424900

C	-5.33515600	3.64368600	2.75050900
H	-5.63249600	4.68873700	2.72893100
C	-4.61881400	3.14781700	3.80639300
H	-4.33958000	3.79060200	4.63822700
C	-5.34834800	1.45729500	1.68996100
H	-5.65685200	0.81502300	0.87303200
C	1.14692900	2.47224900	2.62786900
H	1.15666200	1.39772200	2.83239700
H	2.11225900	2.80501000	2.23892200
H	1.00265000	2.98505800	3.59285000
C	-0.03557400	5.98360200	-0.65529400
C	-0.93609500	6.83635300	0.00884100
C	0.88653300	6.58429900	-1.52587900
C	-0.91258100	8.21725100	-0.17509100
H	-1.68344900	6.42244000	0.68049500
C	0.91140600	7.96881200	-1.71749000
H	1.59747800	5.98617900	-2.08268500
C	0.01587600	8.79445100	-1.04237600
H	-1.62342100	8.84140000	0.36016500
H	1.64137200	8.39634800	-2.39963900
H	0.03903000	9.87072900	-1.18878200
C	-1.52317500	3.93555700	-0.89996600
H	-1.58888300	2.87084300	-0.68169300
H	-2.29255500	4.43114100	-0.29132600
C	-1.89069000	4.09875000	-2.36892000
C	-1.94830700	3.01650500	-3.15672800
H	-1.71005800	2.02416800	-2.78440500
H	-2.25605200	3.08645000	-4.19771600
C	-2.29557100	5.45741900	-2.89326000
H	-3.05954400	5.91369500	-2.25003700
H	-1.45819300	6.16137400	-2.92433100
H	-2.70760600	5.37472800	-3.90415300

TS-1-2-5R

l imaginary frequency

H = -5315.349011

G = -5315.549800

E(M06-2X-DCM) = -5316.240220

O	-1.53665000	-1.78437500	-1.33077300
O	-3.12902500	-0.38554200	0.17374800
P	-1.56802500	-0.72420900	-0.10684600
O	-0.95863000	0.63235000	-0.50629900
N	-0.98949900	-1.46393800	1.18514000
S	0.57758300	-1.67812200	1.41030400

C	0.73515700	-3.53913700	1.44223300
F	0.25848800	-4.06017400	0.31062700
F	0.05325800	-4.04659000	2.47664200
F	2.02462700	-3.86107500	1.56927100
C	-0.05830000	4.60748400	-0.34780400
C	0.10965400	4.36130000	1.19194800
H	-0.58197300	5.03495800	1.71900200
H	1.12296100	4.67246600	1.46246200
C	-0.13761800	2.98638800	1.76355600
C	1.05358400	3.81053900	-1.09956500
H	0.75684400	3.60651200	-2.12872900
H	1.93713200	4.44396300	-1.15287100
N	1.50268600	2.56116900	-0.48501600
C	2.80472700	2.38492700	-0.05933100
N	3.10553800	1.07907400	0.20322600
C	4.33123000	0.46812700	0.55921500
C	5.34732700	1.07861200	1.30788800
C	4.49272400	-0.86495800	0.15526200
C	6.50793100	0.36410100	1.60769000
C	5.65784600	-1.56181300	0.46662000
H	3.69789900	-1.35837500	-0.39093200
C	6.68316600	-0.95453900	1.18814900
H	7.59286100	-1.49376300	1.42080900
C	5.79947200	-2.96948700	-0.04386100
C	7.56330400	1.00988200	2.46780900
F	5.97697600	-2.99089100	-1.39666200
F	6.85429800	-3.61171200	0.49656100
F	4.69709700	-3.70885400	0.20341200
F	8.79646800	0.52513000	2.19527400
F	7.60649000	2.34791100	2.30087700
F	7.33758400	0.78435700	3.78406600
S	3.86753800	3.68152600	0.15850900
C	0.27146200	6.13617500	-0.56148700
H	1.21630900	6.32998900	-0.04187300
H	-0.49703000	6.73101200	-0.05157100
H	5.23986400	2.10077400	1.63766800
C	-1.30282500	2.25661800	1.55517300
H	2.36618600	0.38663400	0.05560800
H	-2.18369400	2.76473000	1.17006100
H	-1.50139900	1.45447500	2.26842500
O	1.39631700	-1.27052200	0.23863700
H	0.98883800	1.72396400	-0.75383300
O	1.00783100	-1.22004800	2.73431900
H	-1.03589900	1.49391300	0.49256800

C	-5.62214900	-3.54784000	1.32471400
C	-5.32022700	-3.33835100	-0.01635700
C	-4.55552100	-2.23007700	-0.41499300
C	-4.34156000	-1.55101700	1.92433000
C	-5.16230400	-2.63596000	2.27443700
C	-2.05977800	-1.48086900	-2.59377200
C	-3.43878600	-1.51941900	-2.78293000
C	-3.96753500	-1.05701800	-3.99905500
C	-3.12513100	-0.70331300	-5.04861800
C	-1.74438400	-0.82121800	-4.88173300
C	-1.17460300	-1.19280800	-3.65174200
H	-5.42287400	-2.76589600	3.32056500
H	-1.08044300	-0.60843900	-5.71410500
C	-4.55904200	-2.12138100	-1.93767800
C	-4.77571400	-3.62736800	-2.31720000
H	-3.80813300	-4.14094300	-2.27993000
H	-5.17926700	-3.74963400	-3.32679900
H	-5.90490000	-1.84936600	-4.56847900
H	-5.90517000	-0.10751800	-4.32437100
C	-4.01232800	-1.40202700	0.56410500
H	-6.21764800	-4.40329600	1.63310700
H	-3.53218600	-0.36613700	-5.99859400
C	-5.70083700	-4.18108300	-1.21332900
H	-5.55285800	-5.25229800	-1.03620100
H	-6.76032500	-4.04831800	-1.47365500
C	-5.48078300	-1.04628000	-3.95015300
C	-5.77228500	-1.27510900	-2.45012200
H	-5.78011600	-0.31486400	-1.92131600
H	-6.73214700	-1.76649400	-2.26433300
C	0.30739400	-1.32734900	-3.50609100
C	1.15385400	-0.20869100	-3.71026600
C	0.86735900	-2.59800200	-3.21346900
C	0.66557200	1.09389200	-4.05774500
C	2.58575200	-0.36336200	-3.57297500
C	2.29641000	-2.72754300	-3.04534000
C	1.52029400	2.14191900	-4.29084900
H	-0.40350400	1.24416200	-4.15409700
C	3.43908100	0.76256600	-3.79786600
C	3.11508800	-1.60893100	-3.22428700
C	2.92864600	1.98063200	-4.15632500
H	1.11977600	3.11080100	-4.57832700
H	4.51104500	0.62445000	-3.68104600
H	4.18964500	-1.71424800	-3.09331800
H	3.58851000	2.82555700	-4.32949700

C	-3.91573300	-0.58743100	2.98813200
C	-3.04340400	-1.00707200	4.02187500
C	-4.47610400	0.71512700	3.01103100
C	-2.42488700	-2.29860300	4.04017400
C	-2.73555800	-0.10166700	5.10695800
C	-4.14355200	1.61538300	4.09261000
C	-1.59178300	-2.67380900	5.06051100
H	-2.59582300	-2.97232400	3.20995900
C	-1.86796300	-0.53751500	6.15723300
C	-3.28881200	1.18136300	5.10998500
C	-1.31510000	-1.78844700	6.14064700
H	-1.11756200	-3.65037100	5.03552000
H	-1.65459600	0.15445900	6.96862200
H	-3.05363400	1.85807000	5.92940200
H	-0.65193600	-2.10663200	6.94025100
C	0.65757400	-4.99994900	-2.81093800
H	0.03531700	-5.88804500	-2.73850800
C	0.08335000	-3.79085800	-3.10378000
H	-0.98616700	-3.73545900	-3.27107800
C	2.06019500	-5.10920900	-2.59722000
H	2.49435900	-6.07329600	-2.34755600
C	2.85563000	-4.00259800	-2.71646900
H	3.92769300	-4.06734900	-2.55749200
C	-5.91512800	2.45542500	2.07012400
H	-6.60824900	2.78494100	1.30075300
C	-5.56857800	3.34321900	3.12801400
H	-5.99603400	4.34197000	3.15641100
C	-4.71010500	2.92860800	4.11001200
H	-4.44615800	3.59015000	4.93208200
C	-5.39144900	1.18981500	2.01655700
H	-5.67925000	0.52604800	1.20928900
C	-1.49969200	4.31845300	-0.81143800
C	-2.56577700	5.04597900	-0.24877500
C	-1.81952300	3.36506200	-1.78651900
C	-3.88422500	4.83711000	-0.64627500
H	-2.37068800	5.79075000	0.51845100
C	-3.14113900	3.15101200	-2.19014300
H	-1.04752800	2.75122000	-2.23308200
C	-4.17980700	3.88769100	-1.62731900
H	-4.68095100	5.41664800	-0.18762100
H	-3.34955600	2.39318700	-2.94072500
H	-5.20701600	3.72268800	-1.94076500
C	0.40750800	6.63193200	-1.99189400
C	1.61580600	6.91315000	-2.49580500

H	2.52763600	6.77427400	-1.92023400
H	1.73490500	7.29763400	-3.50614900
C	-0.84820000	6.86483800	-2.79974800
H	-1.39168400	5.93409000	-2.99521400
H	-1.54505000	7.52182900	-2.26224800
H	-0.61367500	7.33221300	-3.76135800
C	0.88744700	2.46653500	2.72147900
H	0.80604400	1.38771500	2.88396700
H	1.90585700	2.73445800	2.42869600
H	0.69858100	2.95852600	3.68957800

TS-1-2-5R-1

l imaginary frequency

H = -5315.347029

G = -5315.548520

E(M06-2X-DCM) = -5316.239617

O	-1.50926900	-1.77920700	-1.33212300
O	-3.09569800	-0.39386500	0.19270600
P	-1.53539900	-0.72950700	-0.09861500
O	-0.92679300	0.62990900	-0.48818800
N	-0.95247300	-1.48159300	1.18406300
S	0.61663300	-1.69154300	1.40230600
C	0.77231000	-3.55231400	1.44770400
F	0.29767600	-4.08075600	0.31847300
F	0.08752500	-4.05289800	2.48397300
F	2.06093400	-3.87522400	1.57981200
C	-0.13837500	4.62016000	-0.34371900
C	0.01679100	4.39848800	1.20149100
H	-0.72363000	5.03146600	1.71128200
H	1.00443500	4.77390200	1.48624500
C	-0.15365000	3.01200700	1.77449700
C	1.04349200	3.90031500	-1.05582900
H	0.83353200	3.77772200	-2.12069600
H	1.91619500	4.54615000	-0.97311900
N	1.47596500	2.62225600	-0.49401000
C	2.78059200	2.41288600	-0.08840800
N	3.05701100	1.10191100	0.16905300
C	4.27758500	0.48592300	0.54041500
C	5.23830000	1.06877700	1.37845900
C	4.48512200	-0.81674700	0.06988900
C	6.39550300	0.35951000	1.69984500
C	5.64475300	-1.51272900	0.40739300
H	3.73060400	-1.28898400	-0.54733000
C	6.61715700	-0.93061200	1.21637200

H	7.52317900	-1.46759200	1.46791400
C	5.83170300	-2.89378100	-0.15794300
C	7.39203700	0.96961200	2.65097500
F	6.00005000	-2.85842100	-1.51133900
F	6.91054000	-3.52044300	0.35243200
F	4.75629500	-3.67879500	0.06755200
F	8.65039800	0.54236000	2.39804600
F	7.39901800	2.31710800	2.58527200
F	7.11934000	0.63929600	3.93590100
S	3.88487800	3.67804300	0.11231900
C	0.06999900	6.16664000	-0.57792600
H	0.97990900	6.45784300	-0.03844800
H	-0.75881400	6.69653300	-0.09767000
H	5.09118500	2.06667700	1.76293900
C	-1.29096000	2.23368100	1.58640100
H	2.31348100	0.41471000	0.01729000
H	-2.19998300	2.70632900	1.22136700
H	-1.44087400	1.42163400	2.30048800
O	1.42831600	-1.29413600	0.22317900
H	0.94249500	1.80078200	-0.77360000
O	1.05402200	-1.22214100	2.72021100
H	-1.01792500	1.48945800	0.51770400
C	-5.55694800	-3.57172600	1.36948200
C	-5.26746500	-3.36231300	0.02567800
C	-4.51539200	-2.24834400	-0.38095200
C	-4.28998400	-1.56191100	1.95475700
C	-5.09857400	-2.65314500	2.31346400
C	-2.04970700	-1.47551800	-2.58733200
C	-3.43046400	-1.52753300	-2.76104500
C	-3.97787700	-1.06916700	-3.97040800
C	-3.15159500	-0.70520800	-5.02918900
C	-1.76792900	-0.80850300	-4.87796800
C	-1.18016500	-1.17615600	-3.65521200
H	-5.35081300	-2.78240100	3.36172500
H	-1.11576300	-0.58743600	-5.71745500
C	-4.53529100	-2.14052300	-1.90344200
C	-4.74222500	-3.64842800	-2.28030300
H	-3.76971900	-4.15324300	-2.25277500
H	-5.15498200	-3.77475400	-3.28568100
H	-5.91338200	-1.88083700	-4.51823300
H	-5.92818400	-0.13901600	-4.27380200
C	-3.97080500	-1.41397500	0.59196300
H	-6.14239000	-4.43174400	1.68437600
H	-3.57307400	-0.37156000	-5.97411000

C	-5.65112900	-4.20999600	-1.16687100
H	-5.49082700	-5.27950400	-0.99010200
H	-6.71434500	-4.08806800	-1.41707700
C	-5.49038000	-1.07357500	-3.90457200
C	-5.76220400	-1.30533900	-2.40152600
H	-5.77204700	-0.34518600	-1.87260100
H	-6.71531800	-1.80535300	-2.20440200
C	0.30521600	-1.29458000	-3.53089600
C	1.13550900	-0.16587900	-3.74668300
C	0.88442700	-2.55933900	-3.25094000
C	0.62619800	1.13226500	-4.07922800
C	2.57123300	-0.30450800	-3.63708700
C	2.31818000	-2.67405600	-3.11396800
C	1.46348600	2.19284100	-4.31893100
H	-0.44583900	1.26928200	-4.15856500
C	3.40702700	0.83277500	-3.87052700
C	3.12104300	-1.54614200	-3.30636000
C	2.87585400	2.04732400	-4.21069400
H	1.04423000	3.15726900	-4.59481200
H	4.48252400	0.70661500	-3.77465900
H	4.19918800	-1.64032000	-3.19878600
H	3.52332600	2.90044600	-4.39083600
C	-3.86885800	-0.59024000	3.01322400
C	-2.98479700	-0.99568300	4.04261700
C	-4.44776100	0.70424000	3.03756900
C	-2.35007300	-2.27931200	4.06059300
C	-2.68232300	-0.08355700	5.12370600
C	-4.12134700	1.61117600	4.11544800
C	-1.50594000	-2.64101300	5.07670700
H	-2.51743800	-2.95721900	3.23314900
C	-1.80255600	-0.50538700	6.16958900
C	-3.25335500	1.19165400	5.12767800
C	-1.23379400	-1.74917700	6.15266200
H	-1.01917400	-3.61132100	5.05103700
H	-1.59328900	0.19129600	6.97802000
H	-3.02266600	1.87319300	5.94437500
H	-0.56160600	-2.05670800	6.94889900
C	0.70829400	-4.96332300	-2.84483000
H	0.09684400	-5.85759900	-2.75808900
C	0.11535300	-3.76022600	-3.12456700
H	-0.95812300	-3.71580500	-3.26757100
C	2.11658300	-5.05858400	-2.66427100
H	2.56616200	-6.01839000	-2.42569500
C	2.89778400	-3.94392600	-2.80071700

H	3.97375800	-3.99803300	-2.66671400
C	-5.92137800	2.42027200	2.10550200
H	-6.62645400	2.73712300	1.34165100
C	-5.58117500	3.31484800	3.15977100
H	-6.02502400	4.30637100	3.19084200
C	-4.70822600	2.91540300	4.13534700
H	-4.44877500	3.58207700	4.95471300
C	-5.37738200	1.16329700	2.04904200
H	-5.66022700	0.49415700	1.24448600
C	-1.54306100	4.23297200	-0.84227200
C	-2.67464100	4.84933700	-0.27440100
C	-1.76442500	3.31155800	-1.87111900
C	-3.96359900	4.55892100	-0.71457300
H	-2.55545200	5.57190400	0.52909500
C	-3.05584100	3.01428100	-2.31767100
H	-0.93452500	2.79118400	-2.33222200
C	-4.16117700	3.63738600	-1.74618900
H	-4.81317800	5.05173200	-0.24965800
H	-3.18845600	2.28356700	-3.11114100
H	-5.16512800	3.40824200	-2.09308200
C	0.18692200	6.63358400	-2.02623300
C	-0.88893500	6.80590300	-2.80307400
H	-1.89716200	6.61004800	-2.45119300
H	-0.79268500	7.15441800	-3.82873300
C	1.57408700	6.96472200	-2.52853100
H	2.02826100	7.75720100	-1.91782200
H	2.25562600	6.10725100	-2.47259600
H	1.54965700	7.31165200	-3.56633300
C	0.91267300	2.53311300	2.70789200
H	0.88153700	1.45061300	2.86399400
H	1.91200800	2.84832900	2.39655100
H	0.72110300	3.00960600	3.68322000

TS-1-2-5R-2

l imaginary frequency

H = -5315.342521

G = -5315.543724

E(M06-2X-DCM) = -5316.233061

O	-1.53212300	-1.97684600	-1.28070600
O	-3.15086600	-0.48499200	0.09370600
P	-1.59100600	-0.87999900	-0.09587400
O	-0.93003800	0.45757900	-0.49999700
N	-1.08203400	-1.58337700	1.24155800
S	0.47416700	-1.72121800	1.58813500

C	0.68625500	-3.57088400	1.73638500
F	0.32174200	-4.16616100	0.59993700
F	-0.06188100	-4.04586200	2.73886900
F	1.97072800	-3.83804000	1.98375200
C	-0.30358800	4.41470400	-0.51265300
C	-0.12490300	4.25937600	1.04636600
H	-0.94712600	4.80232400	1.52877200
H	0.79853300	4.78323200	1.31166000
C	-0.10529900	2.89055100	1.68427800
C	0.94399700	3.77834100	-1.19505500
H	0.75567100	3.61820100	-2.25995300
H	1.79005200	4.45635900	-1.10388200
N	1.41666400	2.52391500	-0.60813200
C	2.74344700	2.33964800	-0.25670400
N	3.02732100	1.04764500	0.08523600
C	4.25111700	0.44753200	0.47260200
C	5.28027200	1.10631500	1.16033100
C	4.39070800	-0.91864100	0.18938700
C	6.43178800	0.40509800	1.51957400
C	5.54480800	-1.60350300	0.56451100
H	3.58699600	-1.44832600	-0.30632100
C	6.58291100	-0.94924000	1.22410900
H	7.48312200	-1.48073900	1.50645300
C	5.66504500	-3.05759700	0.19806400
C	7.50101500	1.10936800	2.31411700
F	5.91311500	-3.21824200	-1.13442000
F	6.67018900	-3.67202500	0.85401200
F	4.52868500	-3.73836700	0.45628900
F	8.72637100	0.58898600	2.07414300
F	7.55709500	2.42782500	2.03437900
F	7.28411500	0.99810400	3.64643800
S	3.85338700	3.61118700	-0.20843700
H	5.18989700	2.15472600	1.39994400
C	-1.17491500	2.00605500	1.62668500
H	2.26761100	0.36484200	0.03223500
H	-2.15520200	2.38032400	1.33912100
H	-1.18742100	1.20283900	2.36516100
O	1.35960200	-1.34459700	0.45786000
H	0.89707600	1.68658900	-0.86487400
O	0.78868500	-1.17180600	2.91051600
H	-0.94264500	1.26221400	0.52193100
C	-5.80301400	-3.50305300	1.27125200
C	-5.43392100	-3.36833500	-0.06271500
C	-4.61393400	-2.30583900	-0.47565700

C	-4.47381500	-1.52878800	1.83941100
C	-5.35089100	-2.56551400	2.19963200
C	-2.00288600	-1.71938300	-2.57640900
C	-3.37375900	-1.73513300	-2.82081500
C	-3.83771800	-1.31652500	-4.07872800
C	-2.94416500	-1.03183800	-5.10597300
C	-1.57544200	-1.17340700	-4.87557400
C	-1.06778700	-1.50227800	-3.60701600
H	-5.66063900	-2.63892100	3.23777100
H	-0.87140200	-1.01297700	-5.68645400
C	-4.54727300	-2.26661100	-1.99978800
C	-4.79625600	-3.78117200	-2.32078500
H	-3.84901900	-4.32268100	-2.21615100
H	-5.15842700	-3.93738500	-3.34126200
H	-5.77464400	-2.07457400	-4.69614800
H	-5.72629000	-0.32378900	-4.52737600
C	-4.08466300	-1.45368000	0.48919200
H	-6.44327000	-4.32140000	1.59048300
H	-3.30320300	-0.72602700	-6.08539800
C	-5.78800900	-4.25389400	-1.23678900
H	-5.68335300	-5.31962200	-1.00430300
H	-6.82972800	-4.10113400	-1.55177200
C	-5.35018400	-1.25826800	-4.09558100
C	-5.71113000	-1.40944700	-2.60119300
H	-5.71140500	-0.42596100	-2.11718700
H	-6.69266800	-1.86362800	-2.43501800
C	0.40318500	-1.67170700	-3.39943900
C	1.28744700	-0.58621300	-3.62070600
C	0.91626400	-2.94577400	-3.04256400
C	0.84434500	0.72089700	-4.00780200
C	2.71128400	-0.78113900	-3.45755700
C	2.33760400	-3.11266400	-2.84379800
C	1.73517600	1.73456500	-4.25540200
H	-0.21906000	0.90143300	-4.11658100
C	3.60342000	0.30929600	-3.70429900
C	3.19492900	-2.02979000	-3.05802000
C	3.13619100	1.53253600	-4.10145100
H	1.36886200	2.70764100	-4.57228500
H	4.66876800	0.14080700	-3.56888100
H	4.26321100	-2.16325400	-2.90691700
H	3.82441700	2.35162500	-4.28750500
C	-4.04106700	-0.54165500	2.87776500
C	-3.24859400	-0.96550800	3.97283000
C	-4.50511800	0.79673500	2.80832400

C	-2.71371400	-2.28993800	4.07906100
C	-2.93430700	-0.03051800	5.03051000
C	-4.16065800	1.72635300	3.86103500
C	-1.95783100	-2.66762400	5.15706600
H	-2.88533400	-2.99011500	3.27107300
C	-2.15102800	-0.46980400	6.14367700
C	-3.39496500	1.28569000	4.94426000
C	-1.68010300	-1.75206200	6.21139600
H	-1.54643100	-3.67182500	5.19970600
H	-1.93289000	0.24546500	6.93321200
H	-3.15258600	1.98552600	5.74176800
H	-1.07973400	-2.07286500	7.05814400
C	0.62275400	-5.31886100	-2.53389500
H	-0.02909100	-6.18239200	-2.43098700
C	0.09273400	-4.10751300	-2.89330500
H	-0.97154100	-4.02690300	-3.08191100
C	2.01773700	-5.46259300	-2.29177100
H	2.41634800	-6.42740300	-1.99080400
C	2.85022200	-4.38852500	-2.44865900
H	3.91713600	-4.47879000	-2.26891400
C	-5.74787600	2.58982200	1.69925600
H	-6.37219500	2.92860600	0.87669400
C	-5.38608700	3.50548000	2.72844200
H	-5.73173300	4.53469700	2.68104400
C	-4.61985900	3.07867300	3.77953300
H	-4.34814100	3.76164100	4.58128500
C	-5.32782900	1.28524000	1.74188700
H	-5.62840700	0.60198600	0.95584600
C	1.05951200	2.56650100	2.56536000
H	1.13387000	1.49718300	2.78348100
H	2.00475900	2.95212000	2.17541200
H	0.88000500	3.08183600	3.52311900
C	-0.36174500	5.93964600	-0.77812200
C	0.56530500	6.62835300	-1.57384200
C	-1.40145900	6.69395700	-0.20496300
C	0.46568900	8.00861400	-1.77585300
H	1.38516900	6.10674200	-2.05335200
C	-1.50151800	8.06920200	-0.39820300
H	-2.15795100	6.20106800	0.39952100
C	-0.56312700	8.73773000	-1.18665300
H	1.20519100	8.50847500	-2.39574000
H	-2.31738800	8.61794000	0.06498400
H	-0.63669600	9.81089400	-1.33969000
C	-1.64681800	3.75592000	-1.00199600

H	-2.39968300	3.88154100	-0.21763600
H	-1.48720200	2.67632800	-1.10290000
C	-2.27229900	4.25910400	-2.29377600
C	-3.52714900	4.72230300	-2.29413000
H	-4.01752000	5.04003200	-3.21103900
H	-4.11250400	4.80081400	-1.38124000
C	-1.49215400	4.15307100	-3.58128000
H	-0.62962400	4.83108100	-3.58704500
H	-1.10761700	3.13585800	-3.73115000
H	-2.11770300	4.40971500	-4.44170900

TS-1-2-5R-3

l imaginary frequency

H = -5315.340901

G = -5315.542095

E(M06-2X-DCM) = -5316.235380

O	-2.13908800	0.01313400	1.91724300
O	-3.31562700	-1.13546900	-0.09930300
P	-2.00566400	-0.27928900	0.33096800
O	-2.00180200	1.11749000	-0.29872600
N	-0.70778700	-1.19893700	0.11658700
S	-0.29582700	-1.96881400	-1.21855000
C	-0.81354000	-3.74095000	-0.91163600
F	-0.51237700	-4.47344300	-1.98485200
F	-0.16821700	-4.23818700	0.14990900
F	-2.12876500	-3.80274900	-0.68832200
C	0.83752800	3.83956900	-0.67086100
C	1.06005000	3.30183400	-2.12984800
H	0.71891000	4.08473400	-2.82168900
H	2.13748300	3.19197400	-2.27375500
C	0.38671100	2.04162200	-2.60867600
C	1.08257600	2.66511400	0.36130800
H	0.12157600	2.35944000	0.77508600
H	1.71185300	3.01151400	1.18126600
N	1.66423300	1.43038700	-0.17534200
C	3.02202700	1.20297800	-0.27832500
N	3.29496100	-0.08947800	-0.65013500
C	4.50773500	-0.78131400	-0.83627600
C	5.76906100	-0.18826600	-0.99437300
C	4.40482300	-2.18155300	-0.89634500
C	6.89312700	-0.99632200	-1.17697700
C	5.54000300	-2.96727600	-1.06771600
H	3.43215800	-2.65177600	-0.80202800
C	6.80024800	-2.38644500	-1.20660200

H	7.68149400	-2.99973000	-1.34608700
C	5.38627900	-4.46274000	-1.01455200
C	8.24620700	-0.34140000	-1.28499200
F	5.18944800	-4.89030400	0.26269000
F	6.47568500	-5.10820100	-1.47958800
F	4.32217800	-4.88880500	-1.72741700
F	9.12089300	-1.10781600	-1.97576200
F	8.79291300	-0.12531600	-0.06575600
F	8.18056600	0.85655100	-1.90388900
S	4.14161100	2.42541200	-0.01897800
H	5.86774800	0.88678700	-0.97299200
C	-0.98930400	1.83832300	-2.59988600
H	2.48398800	-0.70375600	-0.75524200
H	-1.63732000	2.71195500	-2.54567600
H	-1.36468700	1.02342100	-3.21801100
O	1.17835500	-2.03536100	-1.28926400
H	1.08367600	0.60494300	-0.04064000
O	-1.01599100	-1.55197400	-2.43213000
H	-1.35258900	1.37392900	-1.39916900
C	-7.07749400	0.64683300	0.42587000
C	-6.42361800	0.04127600	1.49306200
C	-5.20477100	-0.62685300	1.29781500
C	-5.24195100	0.00186300	-1.06306800
C	-6.50041000	0.58984400	-0.84139500
C	-2.20444500	-1.06113100	2.82586300
C	-3.41186600	-1.73867300	2.99291200
C	-3.43401200	-2.90492500	3.77563700
C	-2.30423900	-3.31374300	4.47422000
C	-1.14484900	-2.54608200	4.39137700
C	-1.05586900	-1.41630800	3.55896700
H	-7.01611700	1.03024400	-1.68921400
H	-0.26716500	-2.82911900	4.96397500
C	-4.83508300	-1.39748900	2.55907600
C	-5.55245700	-0.51847200	3.63957600
H	-5.74120200	-1.06819200	4.56645900
H	-4.90904300	0.33495900	3.88286600
H	-4.72371100	-4.64784200	3.55066500
H	-5.34742100	-3.42627200	4.65359000
C	-4.59658500	-0.57588000	0.04635600
H	-8.02969300	1.15099000	0.56976000
H	-2.32361400	-4.21021500	5.08860400
C	-6.83902800	-0.02142800	2.94634500
H	-7.67126400	-0.72386300	3.09283100
H	-7.17702900	0.94896400	3.32721600

C	-4.79294200	-3.56663200	3.71527700
C	-5.47126200	-2.82821100	2.54294300
H	-6.56261600	-2.80048800	2.61670600
H	-5.21207700	-3.31730700	1.59687000
C	0.22356100	-0.64125300	3.55229400
C	0.25970900	0.66319400	4.10759500
C	1.42318600	-1.27102300	3.13497000
C	-0.89940700	1.32546300	4.62746000
C	1.52356800	1.35857600	4.20996100
C	2.68397300	-0.58075500	3.29093600
C	-0.82324600	2.57925700	5.17631800
H	-1.85416700	0.81300700	4.59893600
C	1.55680100	2.67478000	4.77049300
C	2.69776500	0.71963000	3.80217900
C	0.41903500	3.27263900	5.24184000
H	-1.71976800	3.05082700	5.56993700
H	2.51675500	3.18222200	4.82912200
H	3.64744200	1.24067500	3.89967000
H	0.45929400	4.26772000	5.67640700
C	-4.68222900	-0.00125500	-2.44897600
C	-4.49605700	-1.22486200	-3.14012400
C	-4.43645100	1.23233800	-3.10454400
C	-4.76859900	-2.50210200	-2.55407400
C	-4.04096100	-1.20618500	-4.51180100
C	-4.02064600	1.23428000	-4.48952600
C	-4.56961600	-3.66509500	-3.25028800
H	-5.14543100	-2.54604400	-1.53913500
C	-3.84225500	-2.44238300	-5.20205500
C	-3.82668100	0.01815300	-5.15009300
C	-4.09211100	-3.64032800	-4.59100400
H	-4.78117700	-4.61972100	-2.77633500
H	-3.48873000	-2.40584400	-6.22963600
H	-3.50552200	0.02446400	-6.18980500
H	-3.93547800	-4.57359700	-5.12465800
C	2.63929800	-3.18503100	2.22371000
H	2.63648200	-4.17555300	1.77719700
C	1.45442100	-2.58188100	2.55698400
H	0.51940800	-3.09164700	2.36335400
C	3.88195500	-2.52097900	2.43182100
H	4.80521700	-3.02292200	2.16115600
C	3.89777200	-1.24800300	2.93356500
H	4.83549600	-0.71498500	3.06852500
C	-4.34386100	3.67874400	-3.12517800
H	-4.44884300	4.62577500	-2.60246800

C	-3.97260000	3.67315900	-4.50060500
H	-3.81258100	4.61408100	-5.02007800
C	-3.80803300	2.48255600	-5.15568200
H	-3.51003500	2.46132000	-6.20142500
C	-4.56257100	2.50337600	-2.45242400
H	-4.82267500	2.52892900	-1.40090700
C	1.25241400	1.03958400	-3.30687800
H	2.24368100	0.94373500	-2.86141300
H	0.76983200	0.06239800	-3.38356400
H	1.39768000	1.41575700	-4.33295400
C	1.78563300	5.04008200	-0.43861000
C	2.05622200	5.48868900	0.86505500
C	2.33006400	5.78849200	-1.49291000
C	2.85356300	6.60568200	1.10408700
H	1.64335900	4.96536300	1.72063200
C	3.12812900	6.91096900	-1.25996700
H	2.15632700	5.50412400	-2.52472800
C	3.39955100	7.32513400	0.04123600
H	3.04603700	6.91342900	2.12861200
H	3.54044600	7.45545400	-2.10561800
H	4.02467500	8.19460200	0.22556700
C	-0.64393100	4.37989900	-0.55400200
H	-0.80286900	5.03453100	-1.41871900
H	-1.32351900	3.52949300	-0.65864900
C	-1.07789100	5.14236300	0.68562500
C	-1.29937600	6.46030800	0.62742500
H	-1.11565100	7.03473400	-0.27702200
H	-1.66106900	7.01658400	1.48902100
C	-1.34737400	4.36008000	1.94898200
H	-1.98474300	3.48881200	1.75119900
H	-0.42859000	3.97336400	2.40602000
H	-1.84197200	4.98467600	2.69965200

TS-1-2-5R-4

l imaginary frequency

H = -5315.341709

G = -5315.543591

E(M06-2X-DCM) = -5316.235221

O	-2.14248000	0.15037500	1.89461000
O	-3.32231500	-1.14986900	-0.02412500
P	-2.00872100	-0.26750600	0.33665800
O	-2.00134100	1.07522100	-0.39927500
N	-0.71400500	-1.20595400	0.20066400
S	-0.28128500	-2.04141400	-1.08802600

C	-0.80183500	-3.79614600	-0.69744100
F	-0.48973900	-4.58152800	-1.72940600
F	-0.16706100	-4.23849300	0.39424300
F	-2.11895000	-3.84719000	-0.48419800
C	0.81696300	3.79359300	-0.80805900
C	1.08211800	3.20598400	-2.24065100
H	0.73701900	3.95351000	-2.96846600
H	2.16429100	3.11457300	-2.35950300
C	0.44092300	1.91459500	-2.68048800
C	1.08730100	2.67745000	0.28159600
H	0.14094600	2.40547200	0.74913100
H	1.74339300	3.06445100	1.05911300
N	1.65737800	1.41439500	-0.20065300
C	3.01561400	1.18306800	-0.29406100
N	3.29574300	-0.13107700	-0.56859000
C	4.51019900	-0.82637900	-0.73350400
C	5.77387000	-0.23910700	-0.89333000
C	4.40769800	-2.22880800	-0.75218700
C	6.89889400	-1.05238200	-1.04670200
C	5.54401600	-3.01860800	-0.89123000
H	3.43517400	-2.69695400	-0.64852300
C	6.80576700	-2.44212000	-1.03899600
H	7.68925700	-3.05932300	-1.14324600
C	5.40066100	-4.51200400	-0.78010300
C	8.23613000	-0.40066100	-1.28854400
F	5.31396600	-4.90255900	0.52051100
F	6.45252000	-5.16777500	-1.31387300
F	4.28452600	-4.96221200	-1.39055900
F	9.25928300	-1.18972100	-0.88832300
F	8.35230200	0.77546500	-0.63756300
F	8.43166100	-0.14341800	-2.60375100
S	4.12993500	2.42957600	-0.13545100
H	5.87568800	0.83577900	-0.88166600
C	-0.93213200	1.69373800	-2.69876800
H	2.48731300	-0.75398000	-0.63619100
H	-1.59155800	2.56038800	-2.69521300
H	-1.28304700	0.84892500	-3.29075900
O	1.19380700	-2.10951500	-1.13388300
H	1.07697200	0.59756700	-0.02056100
O	-0.98320500	-1.68646100	-2.33160200
H	-1.32236200	1.27527300	-1.48963400
C	-7.06416400	0.72010700	0.30144100
C	-6.42550000	0.20997200	1.42612100
C	-5.21567900	-0.49138100	1.30417000

C	-5.22714600	-0.08458000	-1.10540600
C	-6.47967700	0.53620500	-0.95038800
C	-2.23191500	-0.84250000	2.88876600
C	-3.45492600	-1.47523900	3.10991600
C	-3.50548200	-2.56519900	3.99469700
C	-2.38706200	-2.93512800	4.73214800
C	-1.20871400	-2.20771300	4.58235000
C	-1.09158200	-1.16051600	3.65128900
H	-6.98375700	0.90142400	-1.83990400
H	-0.33784000	-2.46063500	5.17895500
C	-4.86824600	-1.14631100	2.63558600
C	-5.57511500	-0.15624000	3.62250800
H	-5.77837000	-0.61178600	4.59623700
H	-4.91827500	0.70556400	3.78767700
H	-4.83288000	-4.29282600	3.92540400
H	-5.43357400	-2.96021100	4.90570600
C	-4.59798900	-0.56527700	0.05854000
H	-8.01000400	1.24846500	0.38978700
H	-2.42907500	-3.77120500	5.42549900
C	-6.84940800	0.29364800	2.87600700
H	-7.69470800	-0.37698700	3.08385400
H	-7.17196100	1.30187100	3.15956200
C	-4.87847400	-3.19970700	3.98804200
C	-5.53486000	-2.55908300	2.74796200
H	-6.62565900	-2.50157600	2.81142900
H	-5.28208400	-3.13928000	1.85304200
C	0.21090900	-0.42982400	3.56844400
C	0.29207100	0.92146300	3.98974300
C	1.38657500	-1.13474400	3.20617000
C	-0.84328100	1.67160400	4.43764100
C	1.57805100	1.58254400	4.01776300
C	2.66983700	-0.47417300	3.28888700
C	-0.72571100	2.97571700	4.84302300
H	-1.81331600	1.18868000	4.46779500
C	1.65516200	2.94970400	4.43314900
C	2.72890800	0.86797600	3.67398700
C	0.53766300	3.63269300	4.83121000
H	-1.60543900	3.51573100	5.18299300
H	2.63110400	3.42918600	4.43692800
H	3.69496600	1.36587700	3.71445600
H	0.61009000	4.66820100	5.15206700
C	-4.65207500	-0.22041900	-2.47826600
C	-4.46806300	-1.50442700	-3.05020800
C	-4.38452500	0.94474800	-3.24179200

C	-4.76892600	-2.71899900	-2.35504300
C	-3.98597700	-1.61759900	-4.40789100
C	-3.94201600	0.81378600	-4.61236300
C	-4.57127800	-3.94351600	-2.93685100
H	-5.16707500	-2.66482000	-1.34870800
C	-3.78834300	-2.91428700	-4.97664600
C	-3.74536400	-0.46002900	-5.15221200
C	-4.06582400	-4.04796700	-4.26337500
H	-4.80534900	-4.84786800	-2.38180400
H	-3.41337800	-2.97659200	-5.99533500
H	-3.40292100	-0.55323700	-6.18088900
H	-3.91019000	-5.02817800	-4.70529200
C	2.53164400	-3.15907100	2.45522600
H	2.49001500	-4.18404200	2.09707100
C	1.37059300	-2.49224200	2.74831100
H	0.41823400	-2.98760800	2.60967100
C	3.79680000	-2.51944100	2.59046000
H	4.70058500	-3.07008200	2.35004000
C	3.85784800	-1.20924100	2.98140300
H	4.81309200	-0.69622900	3.05937500
C	-4.28228600	3.37771200	-3.49467300
H	-4.39661700	4.37064000	-3.06767900
C	-3.88294900	3.24034400	-4.85519300
H	-3.70930400	4.12693900	-5.45904300
C	-3.70929000	1.99228600	-5.38966500
H	-3.39043800	1.87048100	-6.42229300
C	-4.51736600	2.27265400	-2.71651300
H	-4.79755300	2.39973800	-1.67764100
C	-0.68727600	4.27362000	-0.72288900
H	-0.89031200	4.84890500	-1.63631200
H	-1.32406800	3.38892200	-0.74772900
C	-1.12329600	5.11412700	0.46953000
C	-1.59567000	4.54403800	1.58468600
H	-1.92922700	5.14491800	2.42753100
H	-1.67952100	3.46718600	1.70046100
C	1.73183400	5.02485200	-0.60234200
C	2.23448400	5.77687500	-1.67487700
C	2.01851100	5.49088400	0.69335600
C	3.00303200	6.92510600	-1.46909800
H	2.04685500	5.47641000	-2.69978300
C	2.78427700	6.63610000	0.90345300
H	1.62308300	4.97322500	1.56014800
C	3.28661900	7.36132000	-0.17743200
H	3.38173800	7.47329900	-2.32793400

H	2.98771200	6.96098900	1.92060200
H	3.88813100	8.25140100	-0.01432400
C	1.33537100	0.89366500	-3.31247800
H	2.32754400	0.85130000	-2.86152900
H	0.87737300	-0.09858200	-3.32703300
H	1.47186200	1.20511900	-4.36106500
C	-1.11846000	6.61498300	0.29373200
H	-1.82208800	6.90348400	-0.50086200
H	-1.42363900	7.12651200	1.21225700
H	-0.13534300	6.99436400	-0.00148200

INT-15

0 imaginary frequency

H = -5393.936535

G = -5394.150226

E(M06-2X-DCM) = -5394.879856

O	-0.11522000	-2.69661500	-0.42022000
O	-2.35518400	-1.45220400	-0.02058800
P	-0.73048900	-1.26066100	0.08862900
O	-0.34506600	-0.12818200	-0.81537900
C	-0.90515200	-3.77780500	-4.38938100
C	-1.83067600	-4.03619000	-3.38323000
C	-1.52572500	-3.74641900	-2.04558300
C	0.64869300	-2.87397300	-2.72258900
C	0.33274800	-3.23656800	-4.04477000
C	-2.98371100	-2.46300500	0.71565600
C	-2.96533900	-3.77340800	0.23635400
C	-3.44400200	-4.80925200	1.05474000
C	-4.03385800	-4.53156300	2.28231300
C	-4.16171500	-3.20260800	2.68243600
C	-3.63976200	-2.14378700	1.92081500
H	1.08122100	-3.07175000	-4.81404800
H	-4.66268800	-2.96379400	3.61587500
C	-2.58949300	-4.33743300	-1.13060500
C	-3.81932700	-4.34179600	-2.10083500
H	-4.27734500	-3.34539000	-2.09320000
H	-4.58699900	-5.06144900	-1.80002300
H	-4.14355600	-6.58270800	0.01978500
H	-2.79456300	-6.89083500	1.10791200
C	-0.33153000	-3.09773800	-1.73670800
H	-1.12902400	-4.01133400	-5.42743700
H	-4.40585000	-5.33263100	2.91611100
C	-3.21830700	-4.63101600	-3.49419200
H	-3.80404500	-4.18853100	-4.30841700

H	-3.17261700	-5.71099500	-3.69302900
C	-3.20746200	-6.15614700	0.40720700
C	-2.23045900	-5.80974500	-0.73579200
H	-1.20081500	-5.83038700	-0.36082100
H	-2.29064500	-6.49687200	-1.58567100
C	-3.88611300	-0.74492000	2.39182000
C	-3.29916700	-0.28187400	3.59362500
C	-4.82274400	0.06273100	1.69853300
C	-2.32553100	-1.03947300	4.32027400
C	-3.67298100	1.01224800	4.11932200
C	-5.17474400	1.36067300	2.22791400
C	-1.77864900	-0.56515700	5.48279000
H	-1.98931000	-1.98436500	3.91382100
C	-3.08725100	1.46379400	5.34380200
C	-4.59757200	1.79528500	3.42415100
C	-2.17008400	0.69805300	6.01056900
H	-1.01831600	-1.14811000	5.99399700
H	-3.38654800	2.43587200	5.72930100
H	-4.87664400	2.76802700	3.82434200
H	-1.72570900	1.05506500	6.93580500
C	2.01640300	-2.34142900	-2.43460900
C	2.45280800	-1.14865000	-3.06312400
C	2.91954600	-3.09626100	-1.64317500
C	1.57399600	-0.30020000	-3.81336000
C	3.83563500	-0.74319900	-2.94898400
C	4.28213400	-2.64028600	-1.48488200
C	2.03727000	0.82132800	-4.45232200
H	0.51916600	-0.54457500	-3.85595800
C	4.28468700	0.41910600	-3.65476200
C	4.70845200	-1.48969900	-2.15351500
C	3.41505200	1.17869700	-4.39217700
H	1.34231000	1.44441600	-5.00814300
H	5.33720800	0.68462700	-3.58710500
H	5.74036700	-1.16352300	-2.04628000
H	3.77065300	2.05506000	-4.92835500
C	-6.38273300	0.44578300	-0.14855900
H	-6.86559300	0.09565000	-1.05726100
C	-5.47843400	-0.35880400	0.49609100
H	-5.25847100	-1.34274600	0.09770100
C	-6.70820100	1.73292700	0.36699900
H	-7.42832000	2.35727500	-0.15505300
C	-6.12193700	2.16932000	1.52483700
H	-6.36971300	3.14420600	1.93821300
C	3.45445700	-5.02104300	-0.23432300

H	3. 14725300	-5. 94630300	0. 24559800
C	4. 78532700	-4. 54904300	-0. 05667900
H	5. 47950900	-5. 11240200	0. 56089000
C	5. 18471500	-3. 39435800	-0. 67188200
H	6. 20178700	-3. 02684600	-0. 55797200
C	2. 55906400	-4. 32475200	-1. 00281900
H	1. 55468100	-4. 70963100	-1. 13080000
C	-2. 02679300	3. 24417100	-1. 74291300
C	-2. 61697100	2. 77428600	-0. 37072400
H	-3. 70159900	2. 69207800	-0. 49601800
H	-2. 25445600	1. 76205400	-0. 16931300
C	-2. 32547600	3. 62865100	0. 86503000
C	-0. 53151000	3. 62902400	-1. 57612000
H	-0. 47742500	4. 41851600	-0. 81973800
H	-0. 15832100	4. 03582100	-2. 52405600
N	0. 34404800	2. 52202000	-1. 16048100
C	1. 57817900	2. 67134500	-0. 70584600
N	2. 25837600	1. 65750500	-0. 16566100
C	3. 58890600	1. 76718900	0. 36438800
C	4. 67108300	1. 90495900	-0. 50144300
C	3. 78169100	1. 69101000	1. 74741500
C	5. 96310400	1. 98665400	0. 02252100
C	5. 07875200	1. 76986500	2. 25335100
H	2. 93359400	1. 55277500	2. 40987000
C	6. 17266700	1. 92057700	1. 39766400
H	7. 17511500	1. 99011700	1. 80179100
C	5. 30634200	1. 64400300	3. 74020600
C	7. 11710300	2. 11557500	-0. 93573300
F	5. 42891000	0. 35448500	4. 11460400
F	4. 28839400	2. 17475000	4. 44485500
F	6. 44118500	2. 27726600	4. 11879100
F	6. 92714600	3. 13522900	-1. 80252700
F	7. 26398200	0. 99531800	-1. 69103200
F	8. 28772200	2. 32589300	-0. 30470500
S	2. 43119600	4. 23319900	-0. 73119300
H	4. 50316700	1. 93553000	-1. 57199800
H	1. 79232400	0. 75298800	0. 00584200
H	-0. 03907600	1. 55499100	-1. 12373400
C	-3. 14477600	4. 64382400	1. 18868800
H	-3. 99732300	4. 82044400	0. 53565200
H	1. 51391200	4. 87860200	-1. 47214000
N	-0. 41468200	-1. 18580700	1. 66913700
S	1. 04870400	-0. 94111300	2. 22625900
O	1. 08182100	0. 05352000	3. 30785300

O	2.08134400	-0.80117400	1.16333100
C	1.46095100	-2.56230500	3.05760200
F	1.41744000	-3.56578500	2.17785300
F	0.58474700	-2.81227700	4.04276400
F	2.68816900	-2.49458200	3.58384500
C	-2.15031600	2.16215300	-2.84172900
C	-2.77459900	0.92575100	-2.62983000
C	-1.63290100	2.41265200	-4.12598600
C	-2.88070500	-0.01586100	-3.65660700
H	-3.18623400	0.67139700	-1.66176500
C	-1.74152400	1.47843000	-5.15513000
H	-1.14364500	3.35870200	-4.34420900
C	-2.36843700	0.25238400	-4.92373300
H	-3.35828300	-0.96944800	-3.45117600
H	-1.33825800	1.71116700	-6.13757500
H	-2.45062300	-0.48293200	-5.71934500
C	-2.69871900	4.58702600	-2.21741200
H	-2.41338700	5.36495600	-1.50037300
H	-2.22853000	4.86256500	-3.17302600
C	-4.20917700	4.66592700	-2.40939900
C	-4.87439500	5.67812500	-1.82431100
H	-4.29866000	6.35420800	-1.19084800
C	-1.16175900	3.19742700	1.73509100
H	-1.20736800	3.63387100	2.73494600
H	-1.14964500	2.10860600	1.86129700
H	-0.18742900	3.47568100	1.31226000
C	-4.86472700	3.67986100	-3.34720000
H	-4.29872300	3.59130700	-4.28197800
H	-4.90279200	2.67301900	-2.91711800
H	-5.88658600	3.97149300	-3.60006300
C	-3.06047200	5.57871600	2.36341300
H	-3.95619400	5.49430100	2.99489100
H	-2.18765900	5.40571100	2.99755500
H	-3.02160400	6.62388300	2.02550000
C	-6.33160300	6.03451900	-1.92285800
H	-6.45623200	7.05636700	-2.30695300
H	-6.90347900	5.36363900	-2.56828800
H	-6.80153100	6.01795300	-0.92981800

INT-15'

0 imaginary frequency

H = -5393.957668

G = -5394.166900

E(M06-2X-DCM) = -5394.887196

C	-2.17949700	4.25097800	0.50351100
C	-2.97417200	3.63862000	1.71474700
H	-2.54229100	2.65491600	1.92704900
H	-2.76868500	4.26313400	2.59417700
C	-4.48392700	3.47860300	1.60462900
C	-2.59936300	3.53598100	-0.80378300
H	-2.15196700	4.02542400	-1.67602800
H	-3.68078000	3.61431000	-0.92137300
N	-2.27522900	2.11508400	-0.79916900
C	-2.99236100	1.16486500	-1.44691200
N	-2.44783000	-0.09722700	-1.28390100
C	-2.98660300	-1.35923300	-1.55574800
C	-4.36431000	-1.62636500	-1.63058500
C	-2.08612800	-2.42971800	-1.67889300
C	-4.80884100	-2.92927900	-1.84166800
C	-2.55285500	-3.72704600	-1.88470900
H	-1.01946300	-2.24642700	-1.60001800
C	-3.91731600	-3.99342900	-1.97928400
H	-4.27653200	-5.00020700	-2.15344300
C	-1.57460200	-4.86511000	-1.91310200
C	-6.28735300	-3.21373700	-1.81407400
F	-2.04119600	-5.93235700	-2.59141400
F	-1.28391600	-5.30257000	-0.65391700
F	-0.39258700	-4.51295200	-2.47314700
F	-7.02305700	-2.16078600	-2.21690100
F	-6.70235500	-3.52557700	-0.55601800
F	-6.61255100	-4.26664400	-2.59658800
S	-4.36165700	1.50964100	-2.37366100
H	-5.07415200	-0.81899100	-1.52819200
C	-5.00179900	2.25380600	1.41156700
H	-1.48972900	-0.11278000	-0.93265200
H	-1.37725800	1.84556500	-0.40495500
H	1.55272400	1.51601700	1.77313700
O	0.71075800	-1.67832400	0.91587000
O	2.75830200	-0.74314700	-0.34457000
P	1.38080200	-0.31946900	0.37214500
O	0.35442800	0.43610700	-0.38600200
C	2.64706800	-3.83374900	3.92949700
C	3.08635600	-3.92655100	2.61378300
C	2.36972600	-3.31163700	1.57422500
C	0.80645700	-2.39166100	3.22017400
C	1.48839800	-3.10867800	4.21516900
C	2.77265200	-1.68481700	-1.39799800
C	2.77834200	-3.04364000	-1.09253000

C	2. 70545100	-3. 96178300	-2. 15517300
C	2. 70741300	-3. 53134500	-3. 47698700
C	2. 77708500	-2. 16606400	-3. 75038100
C	2. 79899000	-1. 21052200	-2. 72301500
H	1. 11426900	-3. 06259100	5. 23357300
H	2. 79636300	-1. 81638700	-4. 77830600
C	2. 91296800	-3. 79580400	0. 23208400
C	4. 40492000	-4. 05275400	0. 62530900
H	4. 90956300	-4. 72984700	-0. 07091500
H	4. 94172900	-3. 09730700	0. 62128300
H	1. 84615500	-5. 95834000	-2. 17311900
H	3. 55637200	-5. 90870200	-1. 74098900
C	1. 30953500	-2. 47972300	1. 90887000
H	3. 19476100	-4. 32075000	4. 73216100
H	2. 65025300	-4. 24882000	-4. 29120300
C	4. 32760900	-4. 60188400	2. 06940900
H	4. 23231300	-5. 69622600	2. 07962900
H	5. 21838100	-4. 35699800	2. 65827300
C	2. 60092600	-5. 37621100	-1. 63533200
C	2. 23305700	-5. 15585200	-0. 15571200
H	2. 54587500	-5. 97499100	0. 49786400
H	1. 14779400	-5. 05193800	-0. 06502400
C	2. 88238500	0. 24502100	-3. 07129400
C	4. 13200800	0. 90522000	-2. 99080300
C	1. 73958800	0. 93014400	-3. 54672700
C	5. 33692500	0. 24043800	-2. 59571300
C	4. 22363100	2. 30311600	-3. 34584800
C	1. 84587300	2. 32807100	-3. 90230000
C	6. 53308900	0. 90718200	-2. 53466500
H	5. 29561200	-0. 81425800	-2. 34669700
C	5. 48862800	2. 96408300	-3. 25774800
C	3. 07852100	2. 97622600	-3. 78297600
C	6. 61302900	2. 29052400	-2. 86266000
H	7. 43281400	0. 37586900	-2. 23598000
H	5. 53770100	4. 01776900	-3. 52244400
H	3. 15312600	4. 02740600	-4. 05530700
H	7. 56933100	2. 80316000	-2. 80570000
C	-0. 42022900	-1. 59590400	3. 54160900
C	-1. 67653900	-2. 02132600	3. 03944000
C	-0. 33338000	-0. 44329700	4. 36087300
C	-1. 84044600	-3. 20489900	2. 25101400
C	-2. 86226300	-1. 24898400	3. 33435500
C	-1. 53088900	0. 31369600	4. 65472200
C	-3. 06762300	-3. 57875500	1. 76908600

H	-0.97442700	-3.81944700	2.03328100
C	-4.12270400	-1.66955600	2.80421300
C	-2.75646200	-0.10354900	4.12878900
C	-4.22750200	-2.79758600	2.03576100
H	-3.15192700	-4.47638600	1.16483200
H	-4.99956000	-1.06601900	3.02655900
H	-3.65076100	0.47870500	4.34089500
H	-5.18313300	-3.09516700	1.61462500
C	-0.62445200	0.99496000	-4.16555600
H	-1.58556500	0.50006000	-4.26685300
C	0.46199700	0.30120100	-3.70090100
H	0.36200700	-0.74812100	-3.44626900
C	-0.51621100	2.37475800	-4.50336900
H	-1.39369400	2.90569100	-4.86072900
C	0.68520400	3.01834800	-4.37530100
H	0.78391100	4.06912200	-4.63840900
C	0.95081800	1.16328200	5.68494800
H	1.90619600	1.50469800	6.07242800
C	-0.23297500	1.89846200	5.97827900
H	-0.17537800	2.78642200	6.60207100
C	-1.43599200	1.48268200	5.47400900
H	-2.34900400	2.03315300	5.68874700
C	0.90157400	0.03539400	4.90727000
H	1.81471800	-0.50842200	4.69560900
N	2.03456000	0.62615800	1.61931400
S	3.54442800	0.61021500	2.37733400
C	4.79137200	1.14162500	1.04808600
O	3.90946100	-0.75083900	2.73665900
O	3.50407600	1.70541800	3.33785800
F	5.72040000	1.87725200	1.65727900
F	5.35796800	0.06785900	0.51176300
F	4.19290300	1.87061000	0.10912700
C	-0.66203700	4.12577000	0.75712500
C	-0.12600500	4.09421100	2.05687900
C	0.25241300	4.09946400	-0.31258100
C	1.25360900	4.07095900	2.27971900
H	-0.77921900	4.08978500	2.92136700
C	1.63080600	4.07612800	-0.09681700
H	-0.10470900	4.10233600	-1.33597400
C	2.14146300	4.07492300	1.20179500
H	1.63259000	4.04506900	3.29738100
H	2.30329800	4.04871000	-0.94961400
H	3.21302900	4.06189800	1.37563200
C	-2.56700600	5.77339100	0.35868400

H	-3.61792700	5.80663300	0.05627900
H	-2.51853100	6.21182800	1.36397300
C	-1.76228400	6.65287000	-0.58984100
C	-2.14160900	6.78001700	-1.87310600
C	-6.44649500	1.86726600	1.27572900
H	-6.64335900	1.51420900	0.25446400
H	-6.69838100	1.03764300	1.95052300
H	-7.13748900	2.68989500	1.47939900
C	-1.51856400	7.61140800	-2.95969000
H	-2.22750300	8.36615600	-3.32760600
H	-0.61367200	8.13448600	-2.64008000
H	-1.25644700	6.98721700	-3.82500400
C	-0.62238800	7.42108600	0.03880900
H	-1.01736100	8.15181100	0.75964300
H	0.04848000	6.76074800	0.59760400
H	-0.02180500	7.97027000	-0.69014900
C	-5.34647100	4.71040400	1.80056400
H	-4.86179000	5.42758200	2.47340700
H	-5.54366600	5.24148200	0.86011400
H	-6.32041400	4.46152200	2.23201400
H	-3.02546800	6.22411500	-2.19039000
H	-4.30224000	1.42490100	1.30491800

INT-15' -1

0 imaginary frequency

H = -5393.957668

G = -5394.166910

E(M06-2X-DCM) = -5394.887197

C	-2.18428500	4.24901800	0.50335100
C	-2.97825700	3.63580200	1.71460500
H	-2.54519700	2.65262900	1.92697700
H	-2.77357600	4.26062000	2.59400700
C	-4.48782800	3.47390800	1.60447500
C	-2.60338500	3.53356000	-0.80392500
H	-2.15648800	4.02345000	-1.67617400
H	-3.68488100	3.61069700	-0.92155600
N	-2.27766900	2.11303200	-0.79924100
C	-2.99393500	1.16185400	-1.44659200
N	-2.44802000	-0.09957900	-1.28332600
C	-2.98523300	-1.36221300	-1.55532000
C	-4.36256700	-1.63102500	-1.63071000
C	-2.08341500	-2.43164100	-1.67815700
C	-4.80544700	-2.93448200	-1.84203100
C	-2.54848700	-3.72949800	-1.88421800

H	-1. 01700500	-2. 24706000	-1. 59885300
C	-3. 91261500	-3. 99754500	-1. 97933800
H	-4. 27053900	-5. 00474500	-2. 15364900
C	-1. 56884700	-4. 86637100	-1. 91234000
C	-6. 28368700	-3. 22044400	-1. 81498200
F	-1. 27786600	-5. 30341000	-0. 65307500
F	-0. 38714000	-4. 51280700	-2. 47216800
F	-2. 03398900	-5. 93423600	-2. 59068300
F	-6. 60715700	-4. 27579500	-2. 59490000
F	-7. 02006500	-2. 16930500	-2. 22139300
F	-6. 69953200	-3. 52912800	-0. 55645400
S	-4. 36391200	1. 50487000	-2. 37297000
H	-5. 07340500	-0. 82447100	-1. 52867300
C	-5. 00420300	2. 24843800	1. 41179000
H	-1. 48987500	-0. 11398900	-0. 93206100
H	-1. 37917500	1. 84464500	-0. 40546000
H	1. 55058600	1. 51777200	1. 77259200
O	0. 71255600	-1. 67774100	0. 91619100
O	2. 75897600	-0. 74048600	-0. 34455600
P	1. 38094300	-0. 31832500	0. 37194300
O	0. 35368400	0. 43560700	-0. 38667300
C	2. 65151500	-3. 83046200	3. 93005100
C	3. 09087600	-3. 92293000	2. 61434400
C	2. 37349900	-3. 30902800	1. 57469500
C	0. 80922300	-2. 39062300	3. 22058100
C	1. 49201100	-3. 10670300	4. 21565300
C	2. 77454100	-1. 68232000	-1. 39783800
C	2. 78178800	-3. 04107800	-1. 09212000
C	2. 71003500	-3. 95950000	-2. 15458900
C	2. 71162700	-3. 52929900	-3. 47648400
C	2. 77974400	-2. 16399500	-3. 75012100
C	2. 80042200	-1. 20823200	-2. 72292700
H	1. 11786100	-3. 06090600	5. 23406200
H	2. 79869800	-1. 81448000	-4. 77810800
C	2. 91726200	-3. 79283000	0. 23263500
C	4. 40954000	-4. 04794300	0. 62587600
H	4. 91497600	-4. 72454300	-0. 07025000
H	4. 94519300	-3. 09184600	0. 62168600
H	1. 85297100	-5. 95700900	-2. 17217400
H	3. 56313100	-5. 90538800	-1. 74004400
C	1. 31233900	-2. 47829800	1. 90923600
H	3. 19981300	-4. 31669300	4. 73276800
H	2. 65535100	-4. 24698800	-4. 29057400
C	4. 33289800	-4. 59691600	2. 07006000

H	4.23885900	-5.69136500	2.08047400
H	5.22340200	-4.35090800	2.65886200
C	2.60709100	-5.37394500	-1.63448600
C	2.23896800	-5.15374500	-0.15490000
H	2.55279300	-5.97239500	0.49880800
H	1.15358600	-5.05112900	-0.06419800
C	2.88210600	0.24734000	-3.07149300
C	4.13098800	0.90896100	-2.99124000
C	1.73848200	0.93107400	-3.54692800
C	5.33668000	0.24563700	-2.59605200
C	4.22099500	2.30688900	-3.34657000
C	1.84314000	2.32906100	-3.90274100
C	6.53208800	0.91375200	-2.53522400
H	5.29657200	-0.80904800	-2.34679100
C	5.48525400	2.96930300	-3.25872200
C	3.07507400	2.97862500	-3.78368400
C	6.61044200	2.29710600	-2.86355600
H	7.43243100	0.38353700	-2.23645200
H	5.53311900	4.02298200	-3.52366300
H	3.14845700	4.02984300	-4.05620300
H	7.56616700	2.81083600	-2.80678000
C	-0.41830000	-1.59612200	3.54196100
C	-1.67416800	-2.02282500	3.03977600
C	-0.33263900	-0.44341900	4.36122000
C	-1.83686800	-3.20659300	2.25139200
C	-2.86066500	-1.25164400	3.33461200
C	-1.53091800	0.31236700	4.65503100
C	-3.06364400	-3.58166300	1.76939100
H	-0.97022800	-3.82029900	2.03375300
C	-4.12065100	-1.67345600	2.80438200
C	-2.75604700	-0.10610400	4.12904500
C	-4.22429400	-2.80160200	2.03594500
H	-3.14702600	-4.47940700	1.16517800
H	-4.99811900	-1.07077700	3.02663900
H	-3.65093900	0.47524900	4.34112000
H	-5.17960600	-3.10005600	1.61470900
C	-0.62567400	0.99306200	-4.16557800
H	-1.58621400	0.49702600	-4.26675600
C	0.46161700	0.30061900	-3.70092600
H	0.36286400	-0.74878200	-3.44614000
C	-0.51905700	2.37294000	-4.50356900
H	-1.39718200	2.90281400	-4.86092800
C	0.68162800	3.01793700	-4.37571100
H	0.77909000	4.06878900	-4.63897000

C	0.94989700	1.16443100	5.68536300
H	1.90490800	1.50681700	6.07289100
C	-0.23465000	1.89840500	5.97867100
H	-0.17797400	2.78640800	6.60248600
C	-1.43722600	1.48143500	5.47433900
H	-2.35079200	2.03099800	5.68904500
C	0.90182300	0.03651600	4.90765400
H	1.81552800	-0.50634500	4.69596500
N	2.03345100	0.62845400	1.61888700
S	3.54341300	0.61449800	2.37684500
C	4.78970900	1.14716300	1.04747200
O	3.91013300	-0.74604000	2.73639600
O	3.50177100	1.70980800	3.33718300
F	5.71777200	1.88410900	1.65655900
F	5.35770000	0.07399600	0.51142700
F	4.19037600	1.87517500	0.10832500
C	-0.66669400	4.12534200	0.75698000
C	-0.13071000	4.09438800	2.05677500
C	0.24782500	4.09983400	-0.31266800
C	1.24890200	4.07251100	2.27969800
H	-0.78399700	4.08933600	2.92120600
C	1.62624000	4.07787200	-0.09681400
H	-0.10922100	4.10226300	-1.33608800
C	2.13681900	4.07727600	1.20182000
H	1.62785100	4.04701700	3.29737800
H	2.29880000	4.05105900	-0.94957500
H	3.20838500	4.06529500	1.37571900
C	-2.57323200	5.77106400	0.35864200
H	-3.62425900	5.80341100	0.05650600
H	-2.52487300	6.20950300	1.36392900
C	-1.76954700	6.65132500	-0.59010100
C	-2.14918700	6.77795700	-1.87330700
H	-3.03248500	6.22107500	-2.19046400
C	-6.44839700	1.86002400	1.27602700
H	-6.64466100	1.50626200	0.25488000
H	-6.69926000	1.03033100	1.95111800
H	-7.14046500	2.68184800	1.47925600
C	-1.52713600	7.60987200	-2.96003100
H	-0.62300300	8.13427300	-2.64044900
H	-1.26408200	6.98579000	-3.82515500
H	-2.23709000	8.36352100	-3.32823100
C	-0.63034700	7.42073300	0.03833300
H	-1.02593800	8.15098000	0.75931200
H	0.04137100	6.76106300	0.59688300

H	-0.03052700	7.97062900	-0.69073100
H	-4.30364400	1.42032800	1.30538400
C	-5.35186500	4.70473000	1.80002100
H	-6.32558300	4.45476000	2.23135800
H	-4.86816100	5.42259800	2.47282800
H	-5.54953100	5.23539300	0.85944000

INT-15' -2

0 imaginary frequency

H = -5393.954029

G = -5394.166062

E(M06-2X-DCM) = -5394.881768

C	-3.96031100	2.58701600	0.72528300
C	-3.80419400	3.11484100	-0.74575300
H	-3.03544800	2.50220900	-1.22781100
H	-4.73636800	2.91522600	-1.28673200
C	-3.42509200	4.57441400	-0.96972500
C	-2.78506200	3.13042200	1.58186100
H	-2.92469000	2.86806100	2.63893200
H	-2.78167000	4.21951700	1.53450000
N	-1.47586800	2.67666800	1.13507700
C	-0.33258000	3.39262700	1.31011000
N	0.77820800	2.70796700	0.85605300
C	2.13796400	3.04547800	0.80683000
C	2.73338400	4.12106400	1.48775900
C	2.95900600	2.20677800	0.02830500
C	4.10519600	4.34538800	1.37108500
C	4.32711600	2.44857900	-0.06870400
H	2.51821300	1.37906000	-0.51872800
C	4.91885000	3.52219400	0.59757200
H	5.98217200	3.70941600	0.51552000
C	5.19793300	1.50753600	-0.85133800
C	4.70550100	5.54645700	2.05691100
F	5.63370000	0.47363400	-0.08617500
F	6.29601100	2.11504200	-1.34464600
F	4.54095500	0.95296800	-1.90396800
F	4.62149500	6.65303600	1.28347300
F	6.01717400	5.36033100	2.33340400
F	4.08257600	5.82869700	3.21969200
S	-0.32352100	4.93879900	1.98936200
H	2.12214800	4.77473800	2.09206000
C	-2.19258500	4.86423400	-1.42039800
H	0.58184600	1.77073500	0.50545100
H	-1.38697500	1.68893900	0.90640900

H	-2.15826400	-1.55626400	-0.74110600
O	1.09951100	-0.91554700	-1.48545100
O	0.76915700	-2.60927600	0.44080100
P	0.10420900	-1.33798200	-0.28926000
O	-0.22262900	-0.12125600	0.49272100
C	1.72132900	-3.57572400	-4.65324800
C	2.36632500	-3.77380500	-3.43803600
C	2.26788300	-2.82138400	-2.41054500
C	0.73909700	-1.50638300	-3.80083100
C	0.95345400	-2.42526900	-4.84012800
C	2.07093600	-2.53752500	0.98642800
C	3.16679300	-2.71722300	0.14626600
C	4.45352300	-2.54855400	0.68790000
C	4.63124500	-2.28039200	2.04051100
C	3.51508300	-2.18960000	2.87147800
C	2.21044700	-2.31010600	2.36852800
H	0.47364800	-2.24296200	-5.79705000
H	3.64131700	-2.01020700	3.93505000
C	3.27373100	-3.16109900	-1.31284300
C	3.31176100	-4.71815300	-1.45906900
H	4.21284000	-5.15669500	-1.01924200
H	2.44056100	-5.14335600	-0.94807900
H	6.28388900	-1.92224000	-0.31050700
H	6.01024300	-3.66532800	-0.31506000
C	1.38372300	-1.76259700	-2.57592900
H	1.80980500	-4.30603000	-5.45338700
H	5.62881500	-2.14762000	2.45061900
C	3.19161800	-4.95843500	-2.98202700
H	4.17755000	-4.97767200	-3.46607400
H	2.70490400	-5.91097500	-3.21859200
C	5.50851700	-2.69001100	-0.38450500
C	4.68018100	-2.56961900	-1.67750300
H	5.13261600	-3.07708400	-2.53412900
H	4.56503900	-1.51314100	-1.93614800
C	1.04605000	-2.25614500	3.31197000
C	0.44670400	-3.46898000	3.73133400
C	0.60654600	-1.02105400	3.84318700
C	0.91430800	-4.75409200	3.30727700
C	-0.66559400	-3.43328100	4.65344600
C	-0.50103800	-1.00075600	4.77369700
C	0.31729300	-5.91001700	3.73922100
H	1.76353800	-4.80700300	2.63497900
C	-1.26960300	-4.66137000	5.06753800
C	-1.11487900	-2.20176900	5.13882700

C	-0.79639000	-5.86738700	4.62523800
H	0.69744900	-6.87150300	3.40454200
H	-2.11087700	-4.61407900	5.75511700
H	-1.94755200	-2.18001800	5.83945900
H	-1.25959700	-6.79381200	4.95347400
C	-0.12347400	-0.30141400	-4.01681900
C	0.46455600	0.98900800	-4.02865200
C	-1.51209200	-0.45231300	-4.25898200
C	1.86663600	1.20839100	-3.83969800
C	-0.36486300	2.14997900	-4.26016700
C	-2.32879200	0.72039600	-4.48519100
C	2.40316600	2.46983200	-3.86022000
H	2.51757400	0.35600100	-3.68456100
C	0.23413100	3.44872800	-4.27461500
C	-1.73602800	1.98535200	-4.47422500
C	1.57884000	3.60945900	-4.07780000
H	3.46982600	2.59936200	-3.70588600
H	-0.40851300	4.30782000	-4.45058200
H	-2.35585200	2.86427500	-4.63812900
H	2.02220300	4.60110000	-4.08928200
C	0.78510100	1.40506000	4.06964300
H	1.27060000	2.34099600	3.81121200
C	1.22103000	0.23012900	3.51532300
H	2.05127900	0.23886800	2.81782200
C	-0.31263700	1.42043200	4.97717100
H	-0.64515700	2.36570200	5.39639300
C	-0.93730600	0.25001600	5.31368200
H	-1.77155800	0.24550200	6.01160000
C	-3.51686300	-1.83409500	-4.49664400
H	-3.98302500	-2.81484400	-4.48770500
C	-4.31382500	-0.67612500	-4.72359500
H	-5.38021300	-0.78217500	-4.90342100
C	-3.73198200	0.56329100	-4.71565200
H	-4.32590400	1.45750700	-4.88997500
C	-2.16844200	-1.72557000	-4.27394000
H	-1.58218000	-2.62014100	-4.10111600
N	-1.29660600	-2.09713000	-0.86853400
S	-1.62931800	-3.71455900	-1.22462500
C	-1.59727700	-4.62138200	0.44314000
O	-0.54565200	-4.28624300	-2.00835800
O	-3.02090400	-3.74056200	-1.65682300
F	-1.81615100	-3.77140400	1.44322700
F	-2.56973100	-5.53183500	0.41288000
F	-0.42663900	-5.22729600	0.59326200

C	-4.00594200	1.04540300	0.75069500
C	-4.35664800	0.28801900	-0.37909200
C	-3.77922200	0.34216100	1.94749500
C	-4.50826800	-1.10056900	-0.31023200
H	-4.52818800	0.77173800	-1.33376600
C	-3.91452200	-1.04413300	2.02067100
H	-3.48824500	0.87630100	2.84656400
C	-4.29411700	-1.77449100	0.89408300
H	-4.79048500	-1.65376000	-1.20136500
H	-3.71478000	-1.55209900	2.96024500
H	-4.40969700	-2.85297800	0.94565800
C	-5.26480400	3.11385100	1.44708600
H	-5.09548700	2.99698100	2.52375500
H	-5.33479600	4.19279200	1.26917500
C	-6.60395100	2.46449700	1.13045100
C	-7.19262600	1.70103800	2.06620800
H	-6.65630000	1.56276500	3.00586900
C	-1.59454800	6.21065000	-1.71209900
H	-1.11366200	6.22015500	-2.69962900
H	-2.32013000	7.02804400	-1.68196800
H	-0.81138700	6.43589800	-0.97583100
C	-8.50615000	0.97430000	2.00044800
H	-8.34905100	-0.11061600	2.07706700
H	-9.15101900	1.25599400	2.84401600
H	-9.06185400	1.15975800	1.07761500
C	-7.23416400	2.75808800	-0.21188000
H	-6.75836800	2.18741500	-1.02004800
H	-8.29932400	2.51457300	-0.23324700
H	-7.13351100	3.81935100	-0.46965900
H	-1.50505600	4.03146100	-1.56710200
C	-4.48063600	5.63577900	-0.74203300
H	-4.56199000	5.92540500	0.31419500
H	-4.26903500	6.55053500	-1.30205900
H	-5.47080400	5.28186700	-1.05310900

INT-15⁷-3

0 imaginary frequency

H = -5393.940183

G = -5394.152082

E(M06-2X-DCM) = -5394.874673

O	-1.21914800	-2.76608200	-0.26919700
O	-2.94185700	-0.86990300	0.12204100
P	-1.33563900	-1.17326900	0.11493200
O	-0.72230700	-0.29513900	-0.93535400

C	-2.64705200	-3.89256300	-4.04505400
C	-3.51339800	-3.76973200	-2.96399100
C	-3.02088000	-3.47314900	-1.68428300
C	-0.75861500	-3.33936500	-2.58709900
C	-1.27990400	-3.71123800	-3.83885900
C	-3.78220400	-1.56293900	0.99741100
C	-4.20853400	-2.84804200	0.66059300
C	-4.91883200	-3.60412200	1.60661200
C	-5.29706300	-3.04722400	2.82286900
C	-4.96910900	-1.71854200	3.08695800
C	-4.20131200	-0.95058600	2.19513800
H	-0.58820600	-3.83704200	-4.66669600
H	-5.29250000	-1.25580100	4.01461500
C	-4.13503900	-3.61849300	-0.65495600
C	-5.38194200	-3.31753900	-1.55438200
H	-5.50168800	-2.23107000	-1.63631900
H	-6.30739900	-3.72479800	-1.13566300
H	-6.21033700	-5.14982900	0.80133700
H	-4.94234900	-5.77129900	1.85242400
C	-1.66633000	-3.18957700	-1.52017400
H	-3.02252200	-4.13582300	-5.03591100
H	-5.85120100	-3.62988700	3.55446500
C	-5.02010800	-3.90702400	-2.93503000
H	-5.50592500	-3.37666100	-3.76213400
H	-5.32563300	-4.95981500	-3.01418400
C	-5.16119500	-5.00801200	1.09693400
C	-4.21709200	-5.08836900	-0.12116500
H	-3.21790700	-5.39921700	0.20489900
H	-4.55297000	-5.79348600	-0.88797700
C	-3.93172700	0.48046800	2.54313000
C	-3.14038400	0.79723200	3.67391500
C	-4.58356800	1.51080400	1.81918800
C	-2.43456200	-0.19521800	4.42690100
C	-3.01619500	2.17415100	4.09764600
C	-4.43325600	2.88554500	2.24234400
C	-1.68836400	0.14149400	5.52469600
H	-2.46260300	-1.22371100	4.09090900
C	-2.23759400	2.48086100	5.25797900
C	-3.66120200	3.17816900	3.37068400
C	-1.59565100	1.49482000	5.95636300
H	-1.13950100	-0.62976800	6.05695600
H	-2.16587300	3.52056200	5.56941900
H	-3.57034500	4.21245300	3.69786000
H	-1.00101000	1.74066000	6.83204300

C	0. 71951900	-3. 15981300	-2. 44551700
C	1. 37910800	-2. 14668000	-3. 18541700
C	1. 47133300	-4. 06441200	-1. 65491900
C	0. 67740000	-1. 18301400	-3. 98012400
C	2. 82121300	-2. 05728300	-3. 14987200
C	2. 91115600	-3. 94440300	-1. 60541800
C	1. 34485600	-0. 23364700	-4. 71084100
H	-0. 40508700	-1. 21088500	-3. 99401600
C	3. 48013200	-1. 05203700	-3. 92606500
C	3. 54722600	-2. 95517800	-2. 36208200
C	2. 76785800	-0. 16897800	-4. 69299700
H	0. 78252700	0. 47691500	-5. 31167800
H	4. 56654300	-1. 01116400	-3. 89740800
H	4. 63174900	-2. 88060300	-2. 33200400
H	3. 28350800	0. 57864900	-5. 29065000
C	-6. 06135500	2. 27472300	0. 02425100
H	-6. 70174100	2. 04799700	-0. 82405500
C	-5. 43124100	1. 25700500	0. 69302100
H	-5. 58105400	0. 23286900	0. 37143300
C	-5. 89355900	3. 62830800	0. 43402900
H	-6. 40302100	4. 42268900	-0. 10486800
C	-5. 10335000	3. 91903800	1. 51422300
H	-4. 98169100	4. 94615700	1. 85182700
C	1. 62940700	-5. 98654100	-0. 15466200
H	1. 14595300	-6. 78388700	0. 40326300
C	3. 04422800	-5. 84437300	-0. 08815700
H	3. 62591000	-6. 52729000	0. 52489000
C	3. 66520100	-4. 85366900	-0. 79844300
H	4. 74360200	-4. 73051900	-0. 75668000
C	0. 87266800	-5. 13118800	-0. 91135900
H	-0. 20215700	-5. 26136200	-0. 95316500
C	-1. 00965900	3. 52041700	-1. 31518400
C	-0. 78216200	3. 41827800	0. 22283500
H	-1. 70428000	3. 73453200	0. 72808100
H	-0. 72573200	2. 34931300	0. 46498700
C	0. 38782300	4. 10092200	0. 92021200
C	0. 24115500	2. 99022400	-2. 08602300
H	0. 96848200	3. 79424800	-2. 15735100
H	-0. 05309400	2. 68863800	-3. 09661900
N	0. 91311200	1. 85438700	-1. 43636800
C	2. 20125100	1. 77348600	-1. 15035600
N	2. 65733300	0. 85088500	-0. 29434300
C	4. 00118200	0. 69512100	0. 15035500
C	4. 72028100	1. 77980600	0. 66171300

C	4. 56158800	-0. 58414900	0. 15405200
C	6. 02862500	1. 59196900	1. 10649400
C	5. 86457400	-0. 75878500	0. 62177500
H	3. 97565600	-1. 42760800	-0. 19243400
C	6. 60949100	0. 32439100	1. 08678200
H	7. 61872000	0. 17905700	1. 45128800
C	6. 46136500	-2. 14389700	0. 59621700
C	6. 82758900	2. 77836900	1. 58282000
F	7. 67404300	-2. 18695700	1. 18245900
F	6. 61990000	-2. 58747800	-0. 67905600
F	5. 66947600	-3. 03773600	1. 21958300
F	6. 03773800	3. 72019500	2. 14087900
F	7. 48421900	3. 36962000	0. 55817500
F	7. 75481800	2. 42322000	2. 49535100
S	3. 41501300	2. 83435600	-1. 91948400
H	4. 25532200	2. 75530000	0. 75218200
H	2. 00359400	0. 15102700	0. 11082600
H	0. 31067000	1. 05186800	-1. 14957800
C	1. 13191800	5. 07729600	0. 37450800
H	0. 88069400	5. 41524600	-0. 62798600
H	2. 69380000	3. 02255900	-3. 04041600
N	-0. 87321300	-1. 06282900	1. 65587400
S	0. 62456200	-1. 13866900	2. 15090800
O	0. 93441600	-0. 13567300	3. 17416200
O	1. 62031200	-1. 29371000	1. 04624300
C	0. 70527800	-2. 77855500	3. 04161200
F	0. 39526800	-3. 77848200	2. 21362400
F	-0. 15614400	-2. 78294800	4. 06910300
F	1. 94048200	-2. 96934200	3. 51639700
C	-1. 31580600	4. 95886100	-1. 77918500
C	-0. 84420700	5. 48081500	-2. 99507600
C	-2. 15892600	5. 78180500	-1. 01294200
C	-1. 18385800	6. 76833600	-3. 41906000
H	-0. 21593400	4. 88242400	-3. 64650000
C	-2. 50102800	7. 06611400	-1. 43208300
H	-2. 56516900	5. 41687900	-0. 07562300
C	-2. 01262500	7. 57105900	-2. 63840600
H	-0. 79962300	7. 13722100	-4. 36668300
H	-3. 15207400	7. 67511400	-0. 81010300
H	-2. 27698900	8. 57316900	-2. 96466300
C	-2. 26889600	2. 61208100	-1. 61589400
H	-2. 04033800	1. 60651900	-1. 25309200
H	-3. 08290400	2. 99062300	-0. 98653300
C	-2. 76065100	2. 51236300	-3. 05283100

C	-2.33575200	1.49190400	-3.82041000
H	-1.65401300	0.77731200	-3.35835800
C	-3.79592400	3.52441000	-3.48852000
H	-4.66085400	3.48016800	-2.81251800
H	-3.41570300	4.54975300	-3.44020700
H	-4.15960600	3.34918900	-4.50407000
C	0.57538200	3.57966800	2.32878100
H	1.35305100	4.10847700	2.88395300
H	-0.35970200	3.67285700	2.89696800
H	0.81943500	2.50917800	2.33959900
C	2.28148700	5.82823000	0.99170100
H	2.55607500	5.46780900	1.98611400
H	3.17522900	5.76387800	0.35529900
H	2.04407700	6.89766600	1.07987700
C	-2.71285100	1.16152800	-5.23855100
H	-3.19574300	0.17574600	-5.29109300
H	-3.39134700	1.88998600	-5.68993300
H	-1.82152600	1.10060600	-5.87920000

INT-15' -4

0 imaginary frequency

H = -5393.945293

G = -5394.155970

E(M06-2X-DCM) = -5394.878338

O	-0.56293600	-2.88696500	-0.46530800
O	-2.63689800	-1.36686700	-0.10575000
P	-1.00349300	-1.36632000	-0.03951800
O	-0.52296100	-0.34816300	-1.03360500
C	-1.49276100	-4.01326700	-4.38944900
C	-2.43569400	-4.12700200	-3.37281000
C	-2.09053100	-3.82803600	-2.04701900
C	0.16080100	-3.21476000	-2.76575500
C	-0.20078300	-3.59441100	-4.07094300
C	-3.37093300	-2.26728000	0.67061200
C	-3.51504900	-3.58654000	0.23757700
C	-4.11428000	-4.52438400	1.09385900
C	-4.65762600	-4.13203500	2.31186800
C	-4.61472800	-2.78492800	2.66703800
C	-3.97065000	-1.82637100	1.86692900
H	0.55309000	-3.53432800	-4.85035300
H	-5.07397100	-2.45464300	3.59409500
C	-3.21701400	-4.24371800	-1.10911700
C	-4.44044300	-4.12558100	-2.08048600
H	-4.76178000	-3.07814200	-2.11448700

H	-5.29429600	-4.72659200	-1.75252900
H	-5.03753700	-6.22957600	0.12348800
H	-3.73382000	-6.66832400	1.22208600
C	-0.82854900	-3.30976100	-1.76761400
H	-1.74917700	-4.25635200	-5.41763500
H	-5.12315800	-4.85792700	2.97376300
C	-3.88753500	-4.54541500	-3.46074700
H	-4.41471700	-4.06261300	-4.29163000
H	-3.98088900	-5.62934500	-3.61691500
C	-4.05294800	-5.91253200	0.49534000
C	-3.04541100	-5.73386100	-0.65932800
H	-2.02484300	-5.87099000	-0.28398600
H	-3.19595100	-6.43835500	-1.48330000
C	-4.02999800	-0.39248700	2.29781500
C	-3.36017200	0.02659100	3.47241400
C	-4.87947800	0.50659600	1.60435800
C	-2.46906400	-0.82646000	4.19871500
C	-3.56062100	1.36900500	3.97156300
C	-5.05998800	1.85053500	2.10733200
C	-1.83904500	-0.39511300	5.33569600
H	-2.26376400	-1.81597100	3.81221500
C	-2.89592100	1.77409000	5.17214000
C	-4.40250000	2.24200700	3.27752500
C	-2.06132300	0.91823300	5.83832100
H	-1.14358900	-1.05445800	5.84616600
H	-3.07029800	2.78210800	5.54212000
H	-4.55999500	3.24760800	3.66378600
H	-1.55610900	1.23949900	6.74520100
C	1.56498900	-2.77091000	-2.50071100
C	2.07651600	-1.62274100	-3.15628400
C	2.41408900	-3.55157700	-1.67615100
C	1.26475500	-0.75938000	-3.96287100
C	3.47330300	-1.27811800	-3.01296800
C	3.79596500	-3.16418200	-1.50286500
C	1.79654500	0.32377300	-4.61410800
H	0.20570200	-0.97080200	-4.04618300
C	3.99465000	-0.15153100	-3.72708800
C	4.29145800	-2.04840000	-2.18273000
C	3.18452100	0.62768900	-4.50971100
H	1.15398900	0.95817000	-5.21950600
H	5.05607500	0.06642500	-3.63342700
H	5.33609600	-1.76935000	-2.06124200
H	3.59413000	1.47606400	-5.05184600
C	-6.44273100	1.02432700	-0.20606200

H	-6.98841700	0.71197600	-1.09237800
C	-5.61381500	0.13742400	0.43135300
H	-5.51295000	-0.87108500	0.04728700
C	-6.60444600	2.35113200	0.28550800
H	-7.27042600	3.03947700	-0.22801100
C	-5.93208100	2.74655400	1.41153000
H	-6.06173500	3.75026700	1.81110800
C	2.81999100	-5.46796100	-0.21436100
H	2.45574500	-6.36423300	0.28049600
C	4.17175600	-5.06451800	-0.02516600
H	4.82460400	-5.65026800	0.61617900
C	4.64299800	-3.94709700	-0.65816400
H	5.67625500	-3.63197000	-0.53367500
C	1.97608000	-4.74213700	-1.01315500
H	0.95388300	-5.07399900	-1.15051300
C	-1.75911500	3.49015700	-1.08283900
C	-1.65818000	3.46248200	0.47166000
H	-2.66366500	3.60160700	0.88936800
H	-1.40393100	2.43423900	0.75376300
C	-0.71694800	4.38794900	1.23653400
C	-0.35985600	3.23372900	-1.71387900
H	0.22284000	4.15033600	-1.75155600
H	-0.49396700	2.88436300	-2.74329600
N	0.44671700	2.21606100	-1.02387300
C	1.69214100	2.33953500	-0.59383900
N	2.37908800	1.26524300	-0.19141600
C	3.72824300	1.27793300	0.29406000
C	4.77250700	1.41783900	-0.61514700
C	3.98258300	1.07626100	1.65352600
C	6.09255500	1.36504500	-0.16146400
C	5.30566600	1.03707800	2.09190800
H	3.15816200	0.94404100	2.34665000
C	6.36479900	1.17892600	1.19088500
H	7.38873600	1.14513800	1.54273700
C	5.60273900	0.78170800	3.54930600
C	7.19951200	1.45647500	-1.17680200
F	5.71407000	-0.53851800	3.80695600
F	4.63435800	1.26835100	4.34884500
F	6.76997200	1.35676800	3.92117600
F	8.41730800	1.52358800	-0.60703200
F	7.05562400	2.53832300	-1.97288500
F	7.19892700	0.37294000	-1.99891900
S	2.53530100	3.90808400	-0.50234400
H	4.55290600	1.53669100	-1.67064600

H	1.91421500	0.34694100	-0.12461100
H	0.05591400	1.24870200	-1.01416400
C	-0.33858800	5.60835800	0.80201500
H	-0.72016500	5.94697500	-0.15833900
H	1.41600100	4.56751100	-0.07692000
N	-0.63283600	-1.21951200	1.52442600
S	0.86022700	-1.14737500	2.04702500
O	1.04732600	-0.09715200	3.06085400
O	1.88627200	-1.21815900	0.97069200
C	1.07372100	-2.75440200	2.97630100
F	0.19186400	-2.83047200	3.98489900
F	2.30902000	-2.81249700	3.48338000
F	0.88521800	-3.79352400	2.16041800
C	-2.34468600	4.81058100	-1.61952400
C	-1.83021100	5.47176000	-2.74655100
C	-3.48525000	5.36654000	-1.01340900
C	-2.41660900	6.64252200	-3.23621200
H	-0.96878800	5.07721600	-3.27462100
C	-4.07222000	6.53356000	-1.49778600
H	-3.93459700	4.87681700	-0.15518500
C	-3.53919000	7.18292300	-2.61315000
H	-1.99058100	7.12655000	-4.11125900
H	-4.95141400	6.93600900	-1.00115600
H	-3.99520100	8.09373300	-2.99126900
C	-2.73890600	2.30706100	-1.46372600
H	-2.30960300	1.38408500	-1.06353300
H	-3.66989100	2.47668900	-0.91022200
C	-3.06978600	2.08988900	-2.93458300
C	-2.38190500	1.16546600	-3.63013600
H	-1.61542000	0.60693200	-3.09315600
C	-4.23895100	2.86877200	-3.49547400
H	-4.03832700	3.94414800	-3.54265500
H	-4.51995700	2.53865700	-4.49861700
H	-5.11558700	2.74280000	-2.84603900
C	-0.32512700	3.81048700	2.57781700
H	0.28572000	4.48384900	3.18216400
H	-1.22362200	3.56024900	3.15715300
H	0.21897700	2.86344300	2.46189700
C	0.49564700	6.63427600	1.52583200
H	1.30710500	7.00794900	0.88587000
H	-0.11599800	7.51002500	1.78292700
H	0.94525300	6.26132200	2.44896300
C	-2.55560000	0.75035700	-5.06524400
H	-2.78227600	-0.32283200	-5.13057900

H	-3.34769700	1.29400900	-5.58668500
H	-1.62551000	0.90187900	-5.63151700

INT-15-1

0 imaginary frequency

H = -5393.936641

G = -5394.148943

E(M06-2X-DCM) = -5394.877499

O	-0.62640600	-2.46058100	-1.02478900
O	-2.68111100	-1.02663900	-0.33339700
P	-1.05200300	-1.10373800	-0.20219200
O	-0.48598100	0.13443300	-0.82889600
C	-1.35513100	-2.40680800	-5.14924400
C	-2.36546600	-2.73407200	-4.25114400
C	-2.09032200	-2.83980600	-2.88057700
C	0.23129900	-2.21521700	-3.28953600
C	-0.06566200	-2.19149400	-4.66484100
C	-3.47500700	-2.08585900	0.11471200
C	-3.63320100	-3.21286500	-0.69384900
C	-4.30330200	-4.33555100	-0.18154000
C	-4.89576200	-4.30011200	1.07529500
C	-4.83455300	-3.12047400	1.81444100
C	-4.12744800	-1.99454100	1.36047300
H	0.74159900	-1.98021100	-5.35969100
H	-5.33241700	-3.05832200	2.77762200
C	-3.28405800	-3.45237400	-2.16026800
C	-4.44304800	-2.99005300	-3.10615800
H	-4.71763500	-1.96129600	-2.84527300
H	-5.33838700	-3.61174600	-3.00664400
H	-5.23200600	-5.62770300	-1.65381600
H	-4.00213200	-6.43606700	-0.68774400
C	-0.82661700	-2.49840500	-2.40373700
H	-1.55654200	-2.33647700	-6.21538500
H	-5.41442200	-5.16927300	1.47196400
C	-3.82665500	-3.02113800	-4.52266300
H	-4.28062700	-2.28578800	-5.19718300
H	-3.95904200	-4.00416500	-4.99603700
C	-4.25769400	-5.48337000	-1.16563600
C	-3.18715100	-5.01596600	-2.17251300
H	-2.19260100	-5.30711700	-1.81554900
H	-3.31739500	-5.43466800	-3.17528900
C	-4.18965100	-0.74838100	2.18855500
C	-3.57023500	-0.70351700	3.46015100
C	-5.00196000	0.32923200	1.75427200

C	-2.72441700	-1.75217600	3.94404400
C	-3.77803600	0.44217600	4.31742300
C	-5.19094400	1.47360600	2.61690500
C	-2.14108400	-1.68156500	5.18107100
H	-2.51513600	-2.59392000	3.29712300
C	-3.15965700	0.47018500	5.60695400
C	-4.58006000	1.49608400	3.87347400
C	-2.36694700	-0.56144900	6.03061400
H	-1.47813100	-2.47734900	5.50709500
H	-3.33271100	1.33636400	6.24167800
H	-4.73650000	2.35450400	4.52380700
H	-1.89601800	-0.52566600	7.00935600
C	1.64929700	-2.00182300	-2.86333700
C	2.30758000	-0.79175400	-3.19798000
C	2.37652300	-3.05553700	-2.25240600
C	1.62013300	0.33742200	-3.75216700
C	3.73012100	-0.66295800	-2.97618500
C	3.78414300	-2.88256600	-1.97130400
C	2.29507500	1.47139200	-4.12575900
H	0.54254000	0.29333300	-3.85460600
C	4.40035600	0.52874100	-3.40220500
C	4.42642000	-1.70203800	-2.35427600
C	3.70813600	1.56531900	-3.97041900
H	1.74764000	2.31019300	-4.54835700
H	5.47679800	0.58986800	-3.26069200
H	5.49064100	-1.58725400	-2.16104200
H	4.23039900	2.46067900	-4.29798300
C	-6.47945900	1.38300500	0.11154200
H	-6.99585500	1.34957200	-0.84449900
C	-5.69022000	0.32962100	0.49758600
H	-5.58833700	-0.53061700	-0.15414700
C	-6.64243800	2.51824500	0.95661100
H	-7.27267400	3.34366100	0.63617700
C	-6.01707700	2.55434600	2.17427800
H	-6.14435300	3.40700500	2.83749500
C	2.52021100	-5.31020100	-1.31882900
H	2.04380800	-6.25510800	-1.07188300
C	3.89706300	-5.11986700	-1.01323700
H	4.45756600	-5.91587200	-0.53065600
C	4.50857400	-3.94010400	-1.33809700
H	5.56338400	-3.78357500	-1.12515800
C	1.79070600	-4.31858700	-1.92028000
H	0.74653500	-4.49070000	-2.15108200
C	-1.63169300	3.71468100	-0.65238200

C	-2.24820900	2.98284400	0.59987000
H	-3.33395500	3.08989500	0.52682000
H	-2.04319000	1.91239100	0.50161900
C	-1.83149100	3.45358400	1.99160300
C	-0.10761700	3.87371500	-0.48645800
H	0.06023900	4.44238700	0.43363100
H	0.29190400	4.45717900	-1.32323000
N	0.62799000	2.60190200	-0.39231800
C	1.87242000	2.48247400	0.03995400
N	2.41584600	1.29044200	0.29735000
C	3.74424400	1.08784000	0.80162600
C	3.90931100	0.63122800	2.11309000
C	4.84457700	1.29134000	-0.02813800
C	5.19890700	0.39537100	2.58912900
C	6.12858900	1.05088900	0.46486400
H	4.69559900	1.61697500	-1.05111700
C	6.31187400	0.60503800	1.77190300
H	7.30977800	0.42702900	2.15391200
C	7.30092200	1.22573100	-0.46351200
C	5.39166700	-0.13828000	3.98779600
F	8.47601900	1.24629300	0.19413800
F	7.20471700	2.37137600	-1.17361500
F	7.36953600	0.21674000	-1.37154100
F	4.43939900	0.31218800	4.82725200
F	6.59192600	0.23021900	4.49283200
F	5.34877400	-1.48605200	4.01302300
S	2.91737200	3.88745600	0.35941700
H	3.04199600	0.44850100	2.73904900
H	1.83351900	0.43622800	0.28138700
H	0.12169500	1.71109100	-0.59523300
C	-2.53311500	4.42599900	2.60227300
H	-3.38746200	4.83949700	2.06485600
H	2.10655200	4.79308800	-0.21557300
N	-0.76842000	-1.43498400	1.35408800
S	0.69360400	-1.55154600	1.94793200
O	0.83870000	-0.85231900	3.23296900
O	1.77410400	-1.32361700	0.94671500
C	0.84797800	-3.36504400	2.37129700
F	-0.07810800	-3.70871800	3.27978800
F	2.05920100	-3.60065600	2.88580700
F	0.68087700	-4.11769100	1.28173100
C	-2.00233300	2.97397800	-1.95260200
C	-3.25134500	2.34518000	-2.08727600
C	-1.15847500	2.97025300	-3.07396100

C	-3.63702600	1.74384800	-3.28486700
H	-3.94191000	2.30575700	-1.25309000
C	-1.54185400	2.37086700	-4.27543600
H	-0.17989000	3.43526100	-3.02972600
C	-2.78562000	1.75322300	-4.38921400
H	-4.60959300	1.26240500	-3.34741400
H	-0.86201500	2.38979000	-5.12368700
H	-3.08397200	1.28266900	-5.32203400
C	-2.24622800	5.16836800	-0.70281800
H	-3.31965400	5.03024900	-0.87166800
H	-2.14199700	5.59529700	0.30094900
C	-1.69758600	6.16398900	-1.71706200
C	-2.16363000	6.17353200	-2.97709200
H	-2.92383800	5.43457200	-3.22868600
C	-0.69710000	2.70894900	2.66476500
H	0.28917700	2.99946500	2.27950200
H	-0.67525700	2.87431800	3.74396000
H	-0.79187700	1.62827400	2.50883700
C	-0.69792900	7.16523700	-1.17947900
H	-0.29321500	7.82495500	-1.95039100
H	-1.16691300	7.79906600	-0.41385300
H	0.15251700	6.67713300	-0.68423400
C	-2.32084300	5.02291000	3.96582300
H	-3.20073200	4.86160900	4.60434400
H	-1.45107800	4.61585300	4.48681300
H	-2.18626200	6.11128100	3.89645700
C	-1.78468800	7.07627000	-4.11688000
H	-1.44528700	6.48466500	-4.97788700
H	-2.65468800	7.65199900	-4.46176400
H	-0.99365300	7.78877500	-3.86840900

INT-15-2

0 imaginary frequency

H = -5393.936636

G = -5394.149180

E(M06-2X-DCM) = -5394.877445

O	-0.64000800	-2.47644800	-0.98896700
O	-2.68972300	-1.02276000	-0.32447200
P	-1.06132900	-1.10558800	-0.18743600
O	-0.48714000	0.12049100	-0.83012500
C	-1.35973600	-2.48167300	-5.11544200
C	-2.37346900	-2.79063900	-4.21472000
C	-2.10173400	-2.87692800	-2.84210700
C	0.22357300	-2.26921200	-3.25531100

C	-0.07035800	-2.26501400	-4.63149100
C	-3.48982200	-2.07114600	0.13788000
C	-3.65124300	-3.20974400	-0.65364800
C	-4.32778400	-4.32136600	-0.12597700
C	-4.92331800	-4.26391400	1.12859500
C	-4.85859800	-3.07332200	1.84962500
C	-4.14510100	-1.95771900	1.38033000
H	0.73934200	-2.06804100	-5.32769600
H	-5.35868300	-2.99406000	2.81039500
C	-3.29987900	-3.47306700	-2.11537700
C	-4.45468200	-3.01975900	-3.07071700
H	-4.72514200	-1.98595700	-2.82597200
H	-5.35306100	-3.63582500	-2.96387000
H	-5.25898800	-5.63169500	-1.58047500
H	-4.03492600	-6.43069000	-0.59936200
C	-0.83749900	-2.53410600	-2.36759300
H	-1.55853000	-2.42654400	-6.18296600
H	-5.44702800	-5.12447600	1.53719600
C	-3.83536900	-3.07495800	-4.48519000
H	-4.28439600	-2.34769600	-5.17167900
H	-3.97127700	-4.06434700	-4.94409500
C	-4.28512400	-5.48426900	-1.09233200
C	-3.21022500	-5.03710700	-2.10377000
H	-2.21781700	-5.32746300	-1.74024700
H	-3.34025600	-5.47029300	-3.10040000
C	-4.20386000	-0.69884400	2.18920200
C	-3.58812200	-0.63768700	3.46191300
C	-5.00980800	0.37584700	1.73624800
C	-2.74892300	-1.68295800	3.96428300
C	-3.79316600	0.52172600	4.30121000
C	-5.19587000	1.53406000	2.58090000
C	-2.16936600	-1.59661400	5.20209100
H	-2.54157900	-2.53525900	3.33069400
C	-3.17888100	0.56613900	5.59222800
C	-4.58869100	1.57265100	3.83887600
C	-2.39264100	-0.46284000	6.03401200
H	-1.51132200	-2.39056500	5.54222200
H	-3.34977800	1.44260300	6.21326300
H	-4.74305100	2.44150500	4.47570500
H	-1.92483000	-0.41464900	7.01371800
C	1.64185500	-2.05588500	-2.83001200
C	2.30653100	-0.85464900	-3.18343200
C	2.36328800	-3.10316800	-2.20136700
C	1.62497400	0.26917200	-3.75548900

C	3. 72967200	-0. 72972900	-2. 96339100
C	3. 77176900	-2. 93306800	-1. 92278100
C	2. 30580400	1. 39357800	-4. 14685900
H	0. 54716000	0. 22904200	-3. 85713300
C	4. 40614100	0. 45152100	-3. 40823300
C	4. 42044500	-1. 76243300	-2. 32490400
C	3. 71935700	1. 48252000	-3. 99294400
H	1. 76280100	2. 22850900	-4. 58266500
H	5. 48286000	0. 50942500	-3. 26762000
H	5. 48531900	-1. 65042700	-2. 13376400
H	4. 24632600	2. 36978700	-4. 33467600
C	-6. 47789800	1. 41135100	0. 07359900
H	-6. 99189700	1. 36573300	-0. 88323200
C	-5. 69461700	0. 36033200	0. 47778700
H	-5. 59494800	-0. 51014300	-0. 16055800
C	-6. 63773200	2. 56014400	0. 90076100
H	-7. 26311500	3. 38356000	0. 56600000
C	-6. 01551800	2. 61187800	2. 11948000
H	-6. 14056000	3. 47514500	2. 76926900
C	2. 49471600	-5. 34279000	-1. 23043400
H	2. 01319100	-6. 28087600	-0. 96793000
C	3. 87258000	-5. 15486600	-0. 92789300
H	4. 42881200	-5. 94590900	-0. 43235800
C	4. 49047200	-3. 98395400	-1. 27216600
H	5. 54619900	-3. 82973800	-1. 06202200
C	1. 77067200	-4. 35740000	-1. 84849600
H	0. 72564800	-4. 52771900	-2. 07667300
C	-1. 61128500	3. 70722500	-0. 69835400
C	-2. 23102700	2. 99575100	0. 56402600
H	-3. 31633200	3. 10511500	0. 48868100
H	-2. 02934200	1. 92333800	0. 48143700
C	-1. 81394600	3. 48558700	1. 94912100
C	-0. 08639500	3. 86068900	-0. 53523200
H	0. 08460800	4. 44126700	0. 37680100
H	0. 31532300	4. 43052400	-1. 38033900
N	0. 64368200	2. 58695700	-0. 42376000
C	1. 88851600	2. 46883900	0. 00801800
N	2. 42718500	1. 27839800	0. 28242600
C	3. 75696200	1. 07645100	0. 78301400
C	3. 92503400	0. 62070000	2. 09446400
C	4. 85503600	1. 27225100	-0. 05171500
C	5. 21505800	0. 37701000	2. 56482800
C	6. 13966200	1. 02383900	0. 43585000
H	4. 70378500	1. 59216800	-1. 07607700

C	6. 32578500	0. 57687300	1. 74201500
H	7. 32316300	0. 37631600	2. 11450200
C	7. 30880200	1. 17516100	-0. 50062400
C	5. 42054000	-0. 05179000	3. 99700200
F	7. 38163400	0. 13842800	-1. 37650700
F	8. 48507300	1. 22220500	0. 15380900
F	7. 20509600	2. 29744000	-1. 24589700
F	5. 57939400	1. 02138400	4. 80718600
F	6. 53066300	-0. 81156600	4. 13032400
F	4. 37699900	-0. 75641500	4. 46536900
S	2. 93934900	3. 87447000	0. 30498300
H	3. 05885400	0. 43370500	2. 72059600
H	1. 83980800	0. 42721900	0. 28476100
H	0. 13326400	1. 69571600	-0. 61419800
C	-2. 51246300	4. 46982400	2. 54425200
H	-3. 36450200	4. 87839500	1. 99942700
H	2. 13009200	4. 77494900	-0. 28012900
N	-0. 78423400	-1. 41630600	1. 37415300
S	0. 67449200	-1. 52457100	1. 97701800
O	0. 81466300	-0. 80317500	3. 25006800
O	1. 76044700	-1. 31658400	0. 97711200
C	0. 82337300	-3. 33092400	2. 43155700
F	0. 65787100	-4. 10147300	1. 35431200
F	-0. 10602900	-3. 65719800	3. 34297900
F	2. 03266200	-3. 56087400	2. 95356500
C	-1. 98680500	2. 95106800	-1. 98815300
C	-3. 24278500	2. 33490200	-2. 11632900
C	-1. 14054900	2. 92054700	-3. 10721100
C	-3. 63281400	1. 72000800	-3. 30555600
H	-3. 93581300	2. 31661400	-1. 28344900
C	-1. 52825600	2. 30753300	-4. 30041800
H	-0. 15657700	3. 37450200	-3. 06760700
C	-2. 77885600	1. 70274100	-4. 40786500
H	-4. 61084700	1. 24913700	-3. 36314600
H	-0. 84636400	2. 30570500	-5. 14722700
H	-3. 08064000	1. 22172900	-5. 33422600
C	-2. 21777200	5. 16344100	-0. 76883800
H	-3. 29212800	5. 02910900	-0. 93480400
H	-2. 11021900	5. 60418800	0. 22855700
C	-1. 66409400	6. 14108700	-1. 79782500
C	-2. 12915500	6. 13365500	-3. 05822900
H	-2. 89261400	5. 39453900	-3. 29926700
C	-0. 68402000	2. 74576800	2. 63453200
H	-0. 65338700	2. 93821400	3. 70898700

H	-0.79190200	1.66260000	2.50642900
H	0.30290300	3.01465500	2.23573500
C	-0.66003800	7.14555400	-1.27465700
H	-1.12671400	7.79371200	-0.51969200
H	0.18714500	6.66081600	-0.77056200
H	-0.25081700	7.79097700	-2.05522900
C	-2.30020300	5.08660000	3.89894300
H	-3.18044700	4.93532700	4.53945200
H	-1.43099300	4.68672100	4.42634600
H	-2.16493300	6.17372800	3.81350100
C	-1.74512200	7.01722100	-4.21126600
H	-2.61247100	7.59071900	-4.56636700
H	-0.95183000	7.73057900	-3.97264300
H	-1.40665100	6.41107700	-5.06248300

INT-15-3

0 imaginary frequency

H = -5472.495245

G = -5472.714677

E(M06-2X-DCM) = -5473.486173

O	-0.33064700	2.68290400	-0.98245300
O	2.00634400	1.89876600	-0.17840900
P	0.41482200	1.51099300	-0.10503900
O	0.25339600	0.15239300	-0.72124600
C	0.67391500	2.98467100	-5.03767700
C	1.45739400	3.59439100	-4.06270000
C	1.07310100	3.55522700	-2.71451600
C	-0.88691500	2.22926000	-3.30537700
C	-0.50279100	2.34253400	-4.65393100
C	2.43617200	3.12503000	0.34285700
C	2.28446200	4.28527600	-0.41692200
C	2.54680700	5.53097500	0.17578900
C	3.06052500	5.61147000	1.46484000
C	3.33261900	4.43204400	2.15630400
C	3.02471800	3.17010900	1.62166900
H	-1.14572400	1.89996300	-5.40890400
H	3.78019700	4.47453500	3.14485000
C	1.95827300	4.48366700	-1.89419100
C	3.25898000	4.47026800	-2.76759500
H	3.84652800	3.58069900	-2.51065500
H	3.89051700	5.34648700	-2.59136600
H	3.08554200	7.13092900	-1.18679200
H	1.61734500	7.45295200	-0.27061300
C	-0.04449800	2.81188900	-2.33903600

H	0.95856000	3.02199900	-6.08638300
H	3.26453700	6.57524200	1.92450800
C	2.75321000	4.36041600	-4.22290600
H	3.46647700	3.85206800	-4.88214500
H	2.57572200	5.35304200	-4.66013600
C	2.18628500	6.65842500	-0.76684300
C	1.36890100	5.93388800	-1.85713800
H	0.31721500	5.87686500	-1.55404700
H	1.40957800	6.42672600	-2.83363800
C	3.42027000	1.95453000	2.40011200
C	2.79862000	1.66243400	3.63732200
C	4.52201500	1.18092600	1.95509500
C	1.66820900	2.39292300	4.12533900
C	3.30133300	0.57808600	4.45146800
C	5.01155600	0.09824300	2.77799900
C	1.08810000	2.08547000	5.32711600
H	1.24323000	3.17254300	3.50677000
C	2.67315300	0.29836400	5.70595700
C	4.39217100	-0.17006900	4.00199800
C	1.60008100	1.03094300	6.13527200
H	0.21069400	2.63517700	5.65431400
H	3.06913200	-0.51528500	6.30965700
H	4.77394600	-0.97812300	4.62337200
H	1.12602800	0.80414300	7.08649600
C	-2.18584400	1.56155000	-2.98284200
C	-2.38504100	0.20338600	-3.33473300
C	-3.25696700	2.31853100	-2.44351500
C	-1.32896900	-0.63604300	-3.81936300
C	-3.69758400	-0.38674800	-3.19788100
C	-4.54774600	1.69529000	-2.25689300
C	-1.56264000	-1.93460600	-4.19404100
H	-0.32308300	-0.23650200	-3.87124400
C	-3.90468500	-1.73841800	-3.62313200
C	-4.73872100	0.36884500	-2.65253700
C	-2.87093900	-2.49229200	-4.11318600
H	-0.73737700	-2.54232400	-4.55415300
H	-4.90728900	-2.15227900	-3.54457000
H	-5.71717100	-0.08842000	-2.52520700
H	-3.04417100	-3.51510800	-4.43848100
C	6.28753400	0.68480800	0.33349100
H	6.79300800	0.91023400	-0.60191100
C	5.21449200	1.44188200	0.72807100
H	4.88497000	2.26664000	0.10660600
C	6.75867300	-0.38661400	1.14464500

H	7.61645800	-0.97107800	0.82266600
C	6.13765700	-0.66288400	2.33341300
H	6.49577700	-1.46781900	2.97074700
C	-4.19086700	4.39860800	-1.56250400
H	-4.06577200	5.44527300	-1.29865800
C	-5.45043500	3.76991100	-1.35296500
H	-6.27245300	4.33811600	-0.92627600
C	-5.62070100	2.45719200	-1.69786200
H	-6.58007000	1.96518600	-1.55641000
C	-3.13759000	3.70131400	-2.09294700
H	-2.19154800	4.20441700	-2.25188600
C	2.45961200	-3.12692700	-0.98391800
C	2.90436100	-2.33244200	0.29855100
H	3.96778500	-2.10474800	0.20034300
H	2.39631200	-1.36430200	0.29104100
C	2.62777100	-2.97398500	1.65841100
C	0.99605100	-3.63178700	-0.80664400
H	0.98555600	-4.29920000	0.06093600
H	0.71646100	-4.21100000	-1.69486300
N	-0.01303100	-2.58341700	-0.60030000
C	-1.23894500	-2.79542600	-0.14889300
N	-2.06059700	-1.78804600	0.15674700
C	-3.39000100	-1.95949200	0.67505600
C	-4.40855300	-2.40833300	-0.16255400
C	-3.65070700	-1.63187000	2.00901600
C	-5.70108800	-2.55462700	0.34650500
C	-4.94810800	-1.77602600	2.49886800
H	-2.85866700	-1.24650900	2.64235100
C	-5.97584800	-2.24127400	1.67535300
H	-6.97866200	-2.35622800	2.06782200
C	-5.25246400	-1.37731800	3.92248400
C	-6.78016400	-3.07121100	-0.56746800
F	-5.52632100	-0.06125500	4.02054100
F	-4.21539500	-1.63715800	4.74229600
F	-6.32915600	-2.04460600	4.40036100
F	-6.54846800	-4.35240700	-0.93176000
F	-6.84329800	-2.35237200	-1.71873000
F	-7.99979300	-3.02493600	0.00108300
S	-1.89929700	-4.42487300	0.12849300
H	-4.19154000	-2.62808600	-1.20170600
H	-1.71943300	-0.81629300	0.11331500
H	0.24140300	-1.58827100	-0.75615100
C	3.50051900	-3.77201300	2.31313900
H	-0.87982100	-5.08639200	-0.44561100

N	-0.02364000	1.76732600	1.42446500
S	-1.48932700	1.45807100	1.94548600
O	-1.49160200	0.75994500	3.23879500
O	-2.39738500	0.92264300	0.89686200
C	-2.16468000	3.15689900	2.32719800
F	-2.16649600	3.92055700	1.23150200
F	-1.41313500	3.75082500	3.26722100
F	-3.41587100	3.04812100	2.78578300
C	2.53251200	-2.28390300	-2.27652600
C	2.84884400	-0.91958100	-2.28929400
C	2.27147000	-2.90158900	-3.51384500
C	2.90196200	-0.20276400	-3.48797100
H	3.05967700	-0.38863400	-1.37018800
C	2.33038900	-2.19203100	-4.71197000
H	2.03691200	-3.96208500	-3.55466500
C	2.64534800	-0.83104500	-4.70425000
H	3.13442000	0.85768300	-3.45899300
H	2.13487900	-2.70420900	-5.65079300
H	2.68700200	-0.27036700	-5.63401600
C	3.26196500	-4.46471200	-1.13032500
H	3.19907800	-4.95689800	-0.15147200
H	2.68550800	-5.11853900	-1.80083200
C	4.72187900	-4.51486900	-1.60688800
C	5.29951700	-5.73577500	-1.67417000
C	1.31804600	-2.56671900	2.32826500
H	1.46890100	-2.30568000	3.37986100
H	0.88796500	-1.68187100	1.85305600
H	0.55354700	-3.35760000	2.30545400
C	5.44507400	-3.24992200	-2.01954000
H	5.13812700	-2.91298900	-3.01677100
H	5.24534200	-2.41682000	-1.34102400
H	6.52744400	-3.38986000	-2.03709300
C	3.18536600	-4.36776200	3.67078400
H	3.67236200	-3.79326300	4.47303700
H	2.11754000	-4.40643800	3.89502800
H	3.57828100	-5.39032700	3.74048900
C	6.70277100	-6.01216200	-2.16493100
H	6.67579300	-6.70701400	-3.01646500
H	7.25058900	-5.12600600	-2.48767600
H	7.29588500	-6.50837900	-1.38350200
C	4.89068300	-4.12722300	1.84148200
H	4.97195800	-5.19638000	1.60058200
H	5.22172400	-3.56616600	0.96815800
H	5.61166500	-3.94191000	2.65002900

C	4.54963500	-6.99511500	-1.27407200
H	3.69217600	-7.19389500	-1.93342400
H	5.20177700	-7.87285600	-1.32220800
H	4.15127900	-6.94059200	-0.25235600

TS-EF-6SS

l imaginary frequency

H = -5393.927348

G = -5394.136040

E(M06-2X-DCM) = -5394.854232

O	-0.77228900	-2.93509400	-0.04408200
O	-2.73270900	-1.25529300	0.23761400
P	-1.09810800	-1.33627400	0.12502400
O	-0.70546300	-0.52767900	-1.07495000
C	-2.11120900	-4.64139700	-3.62630700
C	-2.96745700	-4.50897200	-2.53792200
C	-2.48922400	-4.02305200	-1.31254000
C	-0.27254700	-3.73054500	-2.28748500
C	-0.76950500	-4.28860700	-3.47852900
C	-3.41953900	-1.97543500	1.21486600
C	-3.67819200	-3.33266500	1.01290600
C	-4.23935500	-4.08587100	2.05673900
C	-4.63442500	-3.47764400	3.24259100
C	-4.48048600	-2.09936000	3.37601400
C	-3.87067300	-1.31985500	2.37827400
H	-0.08135500	-4.42507800	-4.30760400
H	-4.82498600	-1.60161200	4.27764700
C	-3.54811600	-4.20548200	-0.23344400
C	-4.84564100	-4.15119900	-1.10879800
H	-5.10633300	-3.10128100	-1.28603700
H	-5.70033900	-4.62993800	-0.62057000
H	-5.35180500	-5.84441700	1.45066300
H	-3.97516400	-6.20794200	2.48618200
C	-1.17769000	-3.56420300	-1.22222100
H	-2.47252900	-5.02657700	-4.57661100
H	-5.07092100	-4.06049600	4.04968500
C	-4.44566800	-4.82130900	-2.44282900
H	-5.01277000	-4.43266300	-3.29655500
H	-4.62342500	-5.90554400	-2.41548900
C	-4.31835600	-5.54881800	1.68059600
C	-3.42017300	-5.61932400	0.42878700
H	-2.37752900	-5.77145100	0.73038600
H	-3.69029600	-6.42746400	-0.25794000
C	-3.81867200	0.16227800	2.59126500

C	-3.04021000	0.69921000	3.64551600
C	-4.67479100	1.00732800	1.83993100
C	-2.11990200	-0.09304600	4.40377000
C	-3.15397100	2.10175100	3.98018300
C	-4.75829700	2.41410900	2.16707800
C	-1.38854400	0.44909000	5.42723800
H	-1.97440600	-1.12897700	4.12754300
C	-2.38910000	2.62291700	5.07212600
C	-4.00686000	2.91980100	3.23279100
C	-1.53347200	1.82117600	5.77850000
H	-0.67377700	-0.16900500	5.96179200
H	-2.50303300	3.67476000	5.32552500
H	-4.10021300	3.97217000	3.49625300
H	-0.95281600	2.22978900	6.60116700
C	1.18079100	-3.39160500	-2.18912200
C	1.73441200	-2.39793900	-3.03330900
C	2.01864200	-4.13163600	-1.31689600
C	0.93810600	-1.58219700	-3.90128900
C	3.16214200	-2.17085300	-3.02939100
C	3.43859600	-3.86582000	-1.29649700
C	1.50804100	-0.64140900	-4.71989500
H	-0.13743200	-1.71015500	-3.89282500
C	3.71780600	-1.18237400	-3.90314900
C	3.97412900	-2.91065500	-2.16468700
C	2.91799200	-0.43930600	-4.72886300
H	0.87734400	-0.03749500	-5.36738500
H	4.79458400	-1.03003900	-3.88522200
H	5.04742200	-2.73760400	-2.16501600
H	3.35187500	0.30991400	-5.38560600
C	-6.33160700	1.36692600	0.07513000
H	-6.94690300	0.97206600	-0.72845900
C	-5.50607200	0.52706500	0.77696300
H	-5.47928200	-0.52734400	0.52851700
C	-6.39652700	2.75403700	0.39077000
H	-7.06191400	3.40431300	-0.17075300
C	-5.63353800	3.25732600	1.41095900
H	-5.69165500	4.31014200	1.67972300
C	2.36960600	-5.85272900	0.38256700
H	1.96860600	-6.62999000	1.02772400
C	3.76212300	-5.56000700	0.42232500
H	4.40855100	-6.10636800	1.10376700
C	4.27913400	-4.59617800	-0.39956200
H	5.33862500	-4.35486500	-0.38031400
C	1.53104800	-5.16665700	-0.45638100

H	0.47542800	-5.41100900	-0.47393600
C	-1.68390200	3.13531600	-1.55558900
C	-1.52947700	3.16401700	-0.00487600
H	-2.46844600	3.52356100	0.44374100
H	-1.45452100	2.13329700	0.35812300
C	-0.45533000	3.96579500	0.67029600
C	-0.30760200	2.76424700	-2.20908200
H	0.24672500	3.66274600	-2.46934300
H	-0.47844400	2.21156100	-3.13557400
N	0.58340500	1.95993200	-1.37017100
C	1.87833600	2.24709400	-1.13063800
N	2.61624200	1.26841800	-0.56800900
C	3.96437800	1.33814900	-0.11421600
C	4.41960600	2.33753200	0.75116800
C	4.82111200	0.30648800	-0.49464400
C	5.74031500	2.31557200	1.19333600
C	6.13987800	0.28905400	-0.03489800
H	4.45151700	-0.47828000	-1.14419700
C	6.61122300	1.29489500	0.80388100
H	7.63471200	1.28168900	1.15799300
C	7.03301000	-0.84947600	-0.45048600
C	6.25094300	3.43019300	2.06824400
F	6.66899300	-2.01391100	0.13549800
F	8.32498900	-0.62906700	-0.13649600
F	6.97370700	-1.06119600	-1.79087100
F	6.81759000	4.41680800	1.33573100
F	7.19250400	2.99516900	2.93366400
F	5.26108800	3.99722900	2.79252200
S	2.55573900	3.80671300	-1.48132800
H	3.74932000	3.11778100	1.08300600
H	2.17280800	0.36122100	-0.36802400
H	0.24812300	0.99815100	-1.18172300
C	0.16821400	5.07522000	0.06274900
H	-0.38798000	5.47979700	-0.78552100
H	1.08774900	4.49805200	-0.56576100
N	-0.55710700	-0.92899100	1.59281400
S	0.98232200	-0.78599900	1.93973100
O	1.25161500	0.43255400	2.72117900
O	1.90087300	-1.07245100	0.80514700
C	1.29485100	-2.19565800	3.12545600
F	0.50671700	-2.08188600	4.20645700
F	2.57019100	-2.16835400	3.52307200
F	1.04364900	-3.36336700	2.53180200
C	-2.21374200	4.46579700	-2.13080000

C	-1.76734400	4.98136600	-3.35849900
C	-3.24384700	5.16775900	-1.47983500
C	-2.29614400	6.15898800	-3.89234500
H	-1.00216800	4.46479300	-3.92753200
C	-3.77446800	6.34404900	-2.00859900
H	-3.66340500	4.78976800	-0.55218300
C	-3.29807500	6.85268800	-3.21743200
H	-1.92073700	6.52774500	-4.84325100
H	-4.56579300	6.86155200	-1.47228100
H	-3.70794700	7.77063100	-3.62951500
C	-2.77817500	2.02481000	-1.82540000
H	-2.40784500	1.08615100	-1.40126000
H	-3.65905300	2.31106500	-1.24128100
C	-3.20900100	1.77967300	-3.26274900
C	-4.32324100	2.36438200	-3.73233500
H	-4.86975800	3.02535700	-3.05930400
C	-2.38164800	0.80879100	-4.08764100
H	-1.79880100	0.14718700	-3.43961200
H	-3.01162800	0.17843300	-4.72416500
H	-1.67649800	1.32135900	-4.75841000
C	-0.07353100	3.48510500	2.02591500
H	0.44221500	2.51248700	1.96984000
H	0.55377200	4.18476100	2.57842700
H	-0.97856700	3.27323800	2.61060300
C	0.92348400	6.13780300	0.86081100
H	1.43228900	6.81490200	0.16852400
H	0.23667100	6.73466000	1.47132000
H	1.68501200	5.70853500	1.51692300
C	-4.91730500	2.23552500	-5.10616900
H	-4.91040700	3.20557700	-5.62309000
H	-4.38184900	1.52240700	-5.73888300
H	-5.96842100	1.91980300	-5.05413400

TS-EF-6SS-1

l imaginary frequency

H = -5393.926102

G = -5394.135507

E(M06-2X-DCM) = -5394.852547

O	-0.91608700	-2.70684800	-0.63826500
O	-2.79582000	-1.19041700	0.32357300
P	-1.18869200	-1.21707700	-0.00643700
O	-0.92129400	-0.10718900	-0.97906900
C	-2.77121500	-3.58216200	-4.28582600
C	-3.45624100	-3.73090400	-3.08395500

C	-2.80114100	-3.51832600	-1.86289500
C	-0.75777100	-2.92100100	-3.05515500
C	-1.42490600	-3.21713500	-4.25737500
C	-3.35389100	-2.13880900	1.18482400
C	-3.63049200	-3.42238800	0.70950200
C	-4.03154800	-4.41552400	1.61861900
C	-4.25788800	-4.11079500	2.95568500
C	-4.10551100	-2.79209000	3.38086700
C	-3.65213600	-1.78283300	2.51642100
H	-0.86937400	-3.13639400	-5.18709200
H	-4.32870400	-2.52489100	4.40971300
C	-3.68238100	-3.98306000	-0.71117600
C	-5.09795700	-3.78338400	-1.35184400
H	-5.38851600	-2.73226000	-1.24076400
H	-5.86614900	-4.39512700	-0.86851200
H	-5.20608700	-6.03616900	0.78579300
H	-3.68891500	-6.56647100	1.50430000
C	-1.49300700	-3.04224700	-1.85994400
H	-3.26796500	-3.75910400	-5.23654200
H	-4.56690900	-4.88081700	3.65801200
C	-4.90146400	-4.11488400	-2.84872700
H	-5.59305800	-3.56448800	-3.49699500
H	-5.06744500	-5.18293400	-3.04771000
C	-4.15275700	-5.75674800	0.92949000
C	-3.44796400	-5.50385400	-0.41876300
H	-2.37113700	-5.67725600	-0.31102300
H	-3.81032200	-6.14498700	-1.22836400
C	-3.60914900	-0.37668100	3.03413400
C	-2.63919900	0.01366000	3.98708500
C	-4.64494100	0.51848500	2.66536900
C	-1.58567700	-0.85538600	4.41482700
C	-2.69501100	1.33918900	4.56424600
C	-4.68198800	1.84521200	3.23907300
C	-0.66310000	-0.45217300	5.34304300
H	-1.50464600	-1.83557600	3.96478200
C	-1.71631500	1.71758900	5.53717600
C	-3.70483600	2.22057200	4.16640700
C	-0.73019100	0.84851500	5.91870100
H	0.14243100	-1.12327300	5.62425700
H	-1.77810900	2.71409200	5.96920800
H	-3.74781600	3.21410400	4.60962100
H	0.00971300	1.14820700	6.65610000
C	0.68740800	-2.53696600	-3.08888200
C	1.09149300	-1.36703700	-3.78052700

C	1. 65990400	-3. 38625800	-2. 50297600
C	0. 16126000	-0. 45484000	-4. 37780700
C	2. 49888400	-1. 05711200	-3. 90231100
C	3. 06066500	-3. 04213500	-2. 59746400
C	0. 58717300	0. 64045500	-5. 08586600
H	-0. 89962300	-0. 64051100	-4. 26071400
C	2. 90023700	0. 10136700	-4. 63965000
C	3. 44255400	-1. 89701900	-3. 30313800
C	1. 97645700	0. 92316100	-5. 22706400
H	-0. 14361000	1. 30147300	-5. 54565600
H	3. 96381800	0. 31054500	-4. 72813300
H	4. 50113300	-1. 66057800	-3. 39516900
H	2. 29665700	1. 79277300	-5. 79480300
C	-6. 71361200	1. 03053900	1. 46380600
H	-7. 51139100	0. 72066300	0. 79394600
C	-5. 70608200	0. 15426200	1. 77447000
H	-5. 71354000	-0. 84409300	1. 35205200
C	-6. 73044700	2. 34423300	2. 01284100
H	-7. 53546300	3. 02681600	1. 75383600
C	-5. 74017400	2. 73575900	2. 87331100
H	-5. 74914000	3. 73079100	3. 31297500
C	2. 29008000	-5. 39509200	-1. 26233300
H	2. 00449000	-6. 31189400	-0. 75366000
C	3. 66418100	-5. 02985900	-1. 32741000
H	4. 41305100	-5. 66226900	-0. 85866500
C	4. 03662900	-3. 88844200	-1. 98299600
H	5. 08155400	-3. 59610100	-2. 03948800
C	1. 32609900	-4. 60506000	-1. 83083600
H	0. 28697600	-4. 90666400	-1. 77533500
C	-1. 22265400	3. 50254100	-1. 71926000
C	-1. 40415600	3. 25015400	-0. 19966000
H	-2. 37243900	3. 65540300	0. 12805300
H	-1. 50072600	2. 17021600	-0. 04783600
C	-0. 39927500	3. 76812500	0. 79654400
C	0. 22412100	3. 05846600	-2. 14864300
H	0. 88244300	3. 92016400	-2. 23024400
H	0. 17663800	2. 58457000	-3. 13479700
N	0. 88555800	2. 10510400	-1. 25171300
C	2. 15473600	2. 23230700	-0. 81651200
N	2. 76467800	1. 11944600	-0. 37452500
C	4. 06272700	0. 98390000	0. 19544500
C	4. 51948800	1. 76804400	1. 25693400
C	4. 85887900	-0. 04811400	-0. 30286800
C	5. 79222200	1. 53965600	1. 77836200

C	6.12471100	-0.27503500	0.23669700
H	4.48081200	-0.66980900	-1.10615100
C	6.60438100	0.52223300	1.27375400
H	7.58989500	0.35006700	1.68942200
C	6.94727600	-1.42190700	-0.28866200
C	6.31746100	2.43291200	2.87191200
F	6.57914700	-2.59982000	0.26007100
F	8.26290000	-1.25782200	-0.03866200
F	6.80514800	-1.56120900	-1.63232600
F	7.00637000	3.48238800	2.36599500
F	7.15937800	1.77252700	3.69612400
F	5.32164700	2.94382300	3.62769900
S	2.93378400	3.78571800	-0.76894500
H	3.88933200	2.53814500	1.67882900
H	2.26254500	0.22028700	-0.42248900
H	0.42496600	1.18344700	-1.17381300
C	0.39878700	4.89866300	0.57003500
H	0.05968200	5.52941400	-0.25358200
H	1.42559200	4.37196700	-0.03556700
N	-0.45658400	-1.23084000	1.43308800
S	1.11554200	-1.29103600	1.59857100
O	1.60927800	-0.29836700	2.56428000
O	1.86251500	-1.40488400	0.31352700
C	1.40393800	-2.94849100	2.41116600
F	0.77715900	-3.00419200	3.59761900
F	2.71331800	-3.12253900	2.61363700
F	0.94464600	-3.93400400	1.63709300
C	-1.47213000	4.95682500	-2.16272400
C	-0.91611600	5.43476100	-3.36273300
C	-2.32696100	5.82419800	-1.46457800
C	-1.18008700	6.72270700	-3.82962100
H	-0.26959000	4.79551600	-3.95658100
C	-2.59147700	7.11555800	-1.92495800
H	-2.80144200	5.50260700	-0.54345400
C	-2.01764200	7.57437800	-3.10962300
H	-0.72761200	7.05770300	-4.75923400
H	-3.25310300	7.76062700	-1.35266600
H	-2.22250100	8.57915800	-3.46851700
C	-2.23181000	2.58061200	-2.51712300
H	-2.00966900	2.75317300	-3.57662300
H	-1.96221300	1.54173900	-2.29460100
C	-3.72187100	2.77643700	-2.29753500
C	-4.41577200	3.55436000	-3.14578000
H	-3.86367400	4.03405200	-3.95505600

C	-4.35825100	2.01799800	-1.15160700
H	-4.32530100	2.57110100	-0.20330600
H	-5.41220100	1.79725100	-1.33984800
H	-3.84683200	1.06611300	-0.97569300
C	-0.31381300	2.97562700	2.06016900
H	0.20398600	2.01953300	1.88947300
H	0.19684000	3.49705100	2.87002700
H	-1.31980800	2.69632900	2.39742400
C	1.08752400	5.67115200	1.69378200
H	1.77707300	6.40356500	1.26334000
H	0.35663900	6.21679600	2.30159300
H	1.66905700	5.02304200	2.35445200
C	-5.88321800	3.87552100	-3.12025000
H	-6.03886500	4.95427200	-2.97806200
H	-6.35954800	3.61769000	-4.07622800
H	-6.42271200	3.35745500	-2.32305500

TS-EF-6SS-2

1 imaginary frequency

H = -5393.925799

G = -5394.134949

E(M06-2X-DCM) = -5394.851836

O	-0.98966300	-2.59885400	-0.76248800
O	-2.77905500	-1.08549200	0.37176700
P	-1.19067600	-1.14308700	-0.03307100
O	-0.93844400	0.01199500	-0.95706200
C	-2.97139500	-3.17914000	-4.40120000
C	-3.63357600	-3.36259500	-3.19128200
C	-2.93770200	-3.25473300	-1.97918500
C	-0.89791200	-2.68297400	-3.19170200
C	-1.60805900	-2.88188000	-4.38941800
C	-3.33493500	-2.07776600	1.18367900
C	-3.68672700	-3.30771700	0.62227100
C	-4.09946000	-4.35092800	1.46817300
C	-4.25802200	-4.14473600	2.83336000
C	-4.02104900	-2.87412100	3.35422100
C	-3.55478200	-1.81957700	2.55279400
H	-1.07248500	-2.77710600	-5.32839300
H	-4.18498400	-2.68201800	4.41058200
C	-3.80812400	-3.75677300	-0.83436900
C	-5.22903000	-3.44860200	-1.41613100
H	-5.46478300	-2.39482000	-1.22750000
H	-6.01250200	-4.05482300	-0.95065700
H	-5.38005400	-5.84383000	0.55721200

H	-3.87008900	-6.50067300	1.18056400
C	-1.60937500	-2.83880000	-1.98539900
H	-3.49917900	-3.27819900	-5.34650800
H	-4.57637400	-4.95401600	3.48559100
C	-5.08996600	-3.68907900	-2.93717200
H	-5.76907200	-3.06249700	-3.52688300
H	-5.31707600	-4.73163700	-3.20038900
C	-4.30988900	-5.62760500	0.68509300
C	-3.63562500	-5.30453400	-0.66293000
H	-2.56506700	-5.53189000	-0.60388700
H	-4.05045400	-5.86623900	-1.50559900
C	-3.41202400	-0.46844700	3.18738900
C	-2.38030400	-0.21587200	4.12237500
C	-4.41709800	0.50416200	2.95784300
C	-1.35751600	-1.17163400	4.41798800
C	-2.33921800	1.05104500	4.81934300
C	-4.36307100	1.76869600	3.65766500
C	-0.37227300	-0.90099800	5.32971900
H	-1.35124100	-2.11005300	3.88044300
C	-1.29624500	1.29143900	5.76842200
C	-3.32303500	2.01024100	4.56106100
C	-0.34113700	0.34388300	6.01972500
H	0.40827600	-1.63390100	5.50796700
H	-1.28366600	2.24649700	6.28911300
H	-3.29608600	2.95679600	5.09840100
H	0.44892500	0.53913400	6.73986900
C	0.56088400	-2.35487300	-3.23838200
C	1.00006700	-1.16990600	-3.88239500
C	1.50954900	-3.26411600	-2.70533300
C	0.09924000	-0.20624300	-4.44287800
C	2.41648800	-0.89878500	-3.99525100
C	2.91963400	-2.95571800	-2.78247700
C	0.55896400	0.89812800	-5.11507600
H	-0.96701600	-0.36157700	-4.33072200
C	2.85346600	0.27314400	-4.68975600
C	3.33497600	-1.78907100	-3.43091800
C	1.95610100	1.14272100	-5.24855100
H	-0.15116900	1.59598200	-5.55235000
H	3.92310500	0.45190100	-4.77180700
H	4.39986200	-1.57720600	-3.50885000
H	2.30313900	2.02051000	-5.78721500
C	-6.52294100	1.21305300	1.93533700
H	-7.37080700	1.00110100	1.28973900
C	-5.53753500	0.27358000	2.09565900

H	-5.61195000	-0.67657600	1.57898300
C	-6.45279000	2.46495600	2.61116200
H	-7.24276300	3.19822200	2.47167500
C	-5.39873000	2.73168500	3.44277500
H	-5.33931600	3.67768600	3.97662300
C	2.08263000	-5.35700200	-1.58184700
H	1.77122600	-6.29376800	-1.12765600
C	3.46591200	-5.02425000	-1.62086900
H	4.19576600	-5.70085600	-1.18504400
C	3.87062700	-3.85843200	-2.21104200
H	4.92283100	-3.58906300	-2.24657500
C	1.14153900	-4.50969100	-2.10438200
H	0.09440000	-4.78567600	-2.06723300
C	-1.19330000	3.61820800	-1.72584800
C	-1.47613500	3.31105200	-0.23213600
H	-2.46478700	3.71080900	0.03931100
H	-1.59410000	2.22711600	-0.13739900
C	-0.51793900	3.75582700	0.84233100
C	0.27230500	3.17089100	-2.08117600
H	0.93909000	4.03009400	-2.09749200
H	0.28070200	2.72853300	-3.08285000
N	0.87422500	2.18307000	-1.17924400
C	2.12851300	2.27325600	-0.69484600
N	2.71819000	1.12983200	-0.30636300
C	4.01032200	0.93984300	0.26164100
C	4.47862500	1.65368000	1.36610900
C	4.78915500	-0.07577300	-0.29572000
C	5.74669300	1.37221600	1.87392400
C	6.04867300	-0.35718400	0.23105400
H	4.40133400	-0.64439300	-1.13286700
C	6.54081700	0.37062100	1.31286100
H	7.52205900	0.15655500	1.71915900
C	6.84970500	-1.48971000	-0.35538600
C	6.28650800	2.19219600	3.01664400
F	6.47801300	-2.68547000	0.14979600
F	8.17100400	-1.34929800	-0.11952800
F	6.68549900	-1.57123600	-1.70121600
F	6.99296800	3.25751600	2.57103400
F	7.11743000	1.47189700	3.80084500
F	5.29949400	2.67557400	3.80127800
S	2.90633300	3.81785800	-0.51968300
H	3.86173000	2.40918600	1.83168700
H	2.22016100	0.23850800	-0.44562800
H	0.39724400	1.26637100	-1.14502100

C	0.30826400	4.88257600	0.72994600
H	0.03218200	5.56554100	-0.07487200
H	1.37205000	4.37252100	0.15433200
N	-0.39661400	-1.25644000	1.36893600
S	1.17021300	-1.47109000	1.47072500
O	1.76499600	-0.65757000	2.53733500
O	1.86700500	-1.47571400	0.15300500
C	1.34714700	-3.23673800	2.06136800
F	0.80352800	-3.37420500	3.28232000
F	2.64340300	-3.55248100	2.13603800
F	0.73780400	-4.08154000	1.22645200
C	-1.38332800	5.09262500	-2.12751700
C	-0.80910900	5.57299500	-3.31814300
C	-2.18280800	5.98438300	-1.39531200
C	-1.01428500	6.88261900	-3.75157900
H	-0.19795000	4.91602500	-3.93012600
C	-2.39136700	7.29687800	-1.82503100
H	-2.65931200	5.66338200	-0.47511200
C	-1.80790400	7.75464200	-3.00562400
H	-0.55283300	7.21907600	-4.67619800
H	-3.01480700	7.96001900	-1.23100000
H	-1.96913800	8.77558600	-3.34013500
C	-2.17001300	2.72611600	-2.59360700
H	-1.83815900	2.83303300	-3.63481400
H	-1.98469900	1.68568100	-2.30623200
C	-3.66179800	3.01754800	-2.53433600
C	-4.43960900	2.35049400	-1.66363000
H	-3.95860200	1.61767100	-1.01439400
C	-4.18968800	3.98734900	-3.56862200
H	-3.97354000	3.61089700	-4.57883500
H	-5.26936200	4.13691400	-3.49934700
H	-3.71134100	4.96914300	-3.49412800
C	-0.51455400	2.88599900	2.05774500
H	-0.20210000	1.86273900	1.80931500
H	0.11396100	3.25739400	2.86677900
H	-1.54171600	2.78571500	2.43678800
C	0.94185300	5.58116900	1.93184300
H	1.67565200	6.31379400	1.58220900
H	0.18640400	6.11760800	2.51734700
H	1.46304000	4.88842500	2.59740700
C	-5.92602500	2.45954200	-1.47276500
H	-6.40790800	1.48661100	-1.64215500
H	-6.16117700	2.74176300	-0.43897400
H	-6.39916800	3.18657200	-2.13757900

TS-EF-6SS-3

l imaginary frequency

H = -5393.920803

G = -5394.126268

E(M06-2X-DCM) = -5394.844566

O	1.79438200	-2.68667100	-0.31510800
O	2.53993200	-0.31366400	-1.02663800
P	1.21827700	-1.18000200	-0.58896100
O	0.62110300	-0.51924200	0.61896800
C	5.16125200	-3.44432700	2.05825800
C	5.30136700	-3.06021700	0.72929300
C	4.17608000	-2.84799200	-0.08234200
C	2.72787900	-3.36494000	1.81451600
C	3.88092000	-3.61470300	2.57934300
C	3.10763900	-0.53665600	-2.28324600
C	3.88167100	-1.67334300	-2.49857300
C	4.21133500	-2.03568200	-3.81328500
C	3.90697700	-1.19020400	-4.87544800
C	3.29930100	0.03909200	-4.60971700
C	2.88021700	0.39249300	-3.31685500
H	3.75461100	-3.93875600	3.60807600
H	3.12294700	0.74195400	-5.41889200
C	4.61096600	-2.59028400	-1.52241500
C	6.05842500	-2.03385700	-1.27441000
H	5.98567800	-0.96657100	-1.03511300
H	6.70005500	-2.13446700	-2.15483700
H	5.96161800	-3.29598100	-4.07924700
H	4.45819400	-4.06440000	-4.57374100
C	2.90323200	-2.94590900	0.48146800
H	6.03400500	-3.61413800	2.68366400
H	4.16294500	-1.46265400	-5.89630400
C	6.57466000	-2.80268800	-0.04311100
H	7.31189100	-2.23405700	0.53508700
H	7.05964200	-3.74565000	-0.33332800
C	4.89533500	-3.38803800	-3.83013000
C	4.69469700	-3.89398900	-2.38062900
H	3.74282400	-4.43115500	-2.30126100
H	5.48967900	-4.56709900	-2.04364000
C	2.31622700	1.75558200	-3.05629300
C	1.06003300	2.13876200	-3.58285300
C	3.10677500	2.69804000	-2.34852400
C	0.21947000	1.23318600	-4.30427300
C	0.58118300	3.48952600	-3.38564000

C	2. 61005500	4. 04081600	-2. 14850600
C	-0. 98739800	1. 63445200	-4. 81364400
H	0. 54029200	0. 20602900	-4. 41875500
C	-0. 68291300	3. 86801900	-3. 93737900
C	1. 36136200	4. 39799300	-2. 66594100
C	-1. 44387700	2. 97147800	-4. 63791800
H	-1. 61138400	0. 91820300	-5. 33952100
H	-1. 02280200	4. 89070400	-3. 78912500
H	0. 99374600	5. 41009100	-2. 50901000
H	-2. 40159200	3. 27242300	-5. 05484000
C	1. 39597600	-3. 60770600	2. 45231100
C	1. 01030200	-2. 83199100	3. 57286600
C	0. 59390000	-4. 69830400	2. 03355400
C	1. 74375500	-1. 67974800	4. 00700400
C	-0. 16871900	-3. 19702200	4. 32539400
C	-0. 61068700	-5. 02057300	2. 76506300
C	1. 37888300	-0. 97831400	5. 12774200
H	2. 59847900	-1. 35295600	3. 42706700
C	-0. 50196000	-2. 45372700	5. 50194900
C	-0. 94938000	-4. 27456600	3. 89781200
C	0. 25276200	-1. 38308000	5. 90112400
H	1. 94879100	-0. 10227900	5. 42180300
H	-1. 37069100	-2. 76644900	6. 07791400
H	-1. 83389900	-4. 55085700	4. 46941900
H	-0. 00697100	-0. 83275000	6. 80182400
C	5. 15121800	3. 33273800	-1. 16306700
H	6. 13784100	3. 07228700	-0. 78888800
C	4. 41030100	2. 39653400	-1. 83635400
H	4. 81985200	1. 40610800	-1. 99738500
C	4. 64568200	4. 64621200	-0. 95132700
H	5. 24371900	5. 37545400	-0. 41146600
C	3. 41149800	4. 98669200	-1. 43514300
H	3. 01467200	5. 98661500	-1. 28477400
C	0. 14234500	-6. 58595100	0. 54885200
H	0. 42595200	-7. 20018800	-0. 30140600
C	-1. 05528200	-6. 88316600	1. 25847300
H	-1. 67556500	-7. 71758500	0. 94254300
C	-1. 41479500	-6. 12289800	2. 33760200
H	-2. 32066100	-6. 34576100	2. 89688100
C	0. 93835300	-5. 53649100	0. 92540000
H	1. 84867900	-5. 33072400	0. 37533100
C	-5. 28673200	0. 33890200	0. 43212000
C	-5. 18096700	0. 09075400	1. 99186600
H	-5. 76176900	0. 87844800	2. 48207300

H	-5.70512600	-0.85209500	2.20180000
C	-3.84233800	0.00615400	2.67319900
C	-4.34770800	1.51656800	0.04232600
H	-4.62330700	2.41397900	0.59455500
H	-4.45832900	1.72571900	-1.02515300
N	-2.91498900	1.29119800	0.28080800
C	-2.08550700	2.13308000	0.92190300
N	-0.76043600	1.90369700	0.82053300
C	0.26840000	2.71963300	1.37030000
C	0.31825400	4.08987700	1.10170800
C	1.27966300	2.11266800	2.11851000
C	1.36103200	4.85578500	1.61782500
C	2.32333700	2.89319500	2.61956500
H	1.25855200	1.04028900	2.27449400
C	2.36812000	4.26556900	2.38223800
H	3.18955800	4.86159400	2.76022300
C	3.38407900	2.24423100	3.46918600
C	1.38693600	6.33890000	1.36066600
F	2.98038100	2.12731300	4.76204700
F	4.52932800	2.95712100	3.48366900
F	3.68284000	0.99852000	3.04314300
F	0.83277400	6.65175700	0.16425500
F	2.64660700	6.82877700	1.36046800
F	0.69785200	7.02405700	2.30022500
S	-2.71218700	3.36277100	1.99392300
H	-0.43342100	4.54849600	0.47165600
H	-0.42022400	0.98824800	0.47302700
H	-2.47219300	0.64905800	-0.39972200
C	-3.57338800	0.95511900	3.66435200
H	-4.46411800	1.44800800	4.06772700
H	-3.26896800	2.01536000	2.88850400
N	0.30829100	-1.39205700	-1.90998800
S	-1.25840300	-1.51695700	-1.81345600
O	-1.95629800	-0.19633600	-1.88884200
O	-1.80091200	-2.44029000	-0.79962500
C	-1.63720300	-2.32195100	-3.45315600
F	-1.16285600	-1.61205200	-4.48513800
F	-2.96809600	-2.41430200	-3.57730100
F	-1.11180700	-3.54644200	-3.49473700
C	-2.88295800	-1.10486300	2.37536500
H	-1.83999100	-0.77373500	2.37781300
H	-2.95633500	-1.84705600	3.18568500
H	-3.07265200	-1.61688800	1.43350500
C	-2.41555000	0.84721000	4.63972800

H	-2.28977100	1.79045500	5.17957000
H	-2.59590500	0.05611700	5.37673400
H	-1.46940100	0.61722400	4.14325300
C	-6.76042800	0.74571800	0.20570200
C	-7.77294200	-0.19772600	0.45425000
C	-7.15970000	2.02778500	-0.19994700
C	-9.12036300	0.12442100	0.31276400
H	-7.50751000	-1.20615000	0.75638700
C	-8.51139400	2.35329600	-0.34983500
H	-6.42785300	2.79877200	-0.41296900
C	-9.49854500	1.40618200	-0.09171900
H	-9.87581300	-0.63067900	0.51345700
H	-8.78463800	3.35563900	-0.66874300
H	-10.54881500	1.65988700	-0.20588500
C	-4.95546600	-0.97561000	-0.36684400
H	-5.25793500	-1.82898900	0.24963100
H	-3.87065600	-1.06372400	-0.47059200
C	-5.57725100	-1.16502000	-1.74501500
C	-6.29509900	-2.27633500	-1.97713600
H	-6.42837800	-2.96895700	-1.14400400
C	-5.28063700	-0.12304500	-2.79693800
H	-5.80348800	0.81883800	-2.58224700
H	-4.20667200	0.08891100	-2.83808300
H	-5.59467700	-0.44092500	-3.79360000
C	-6.94822200	-2.72789800	-3.25269500
H	-6.56345600	-3.71043600	-3.55827400
H	-8.03178400	-2.84617200	-3.11253400
H	-6.79777000	-2.03769600	-4.08634600

TS-EF-6SS-4

l imaginary frequency

H = -5393.920114

G = -5394.126534

E(M06-2X-DCM) = -5394.842497

O	-2.25682100	-2.37477700	0.49589400
O	-2.48610900	0.13256300	1.09783200
P	-1.38165300	-1.00603100	0.67875300
O	-0.70374500	-0.52671200	-0.57174700
C	-5.71698000	-2.56567200	-1.85561000
C	-5.76738100	-2.06716200	-0.55859100
C	-4.62091800	-2.04900000	0.25095500
C	-3.32282200	-2.99667900	-1.58777400
C	-4.50591800	-3.04836500	-2.34594800
C	-3.07813800	0.08365700	2.36127100

C	-4.08280600	-0.84686400	2.61477900
C	-4.48778000	-1.07157400	3.93925800
C	-4.00853100	-0.26937200	4.96972700
C	-3.14267000	0.78154800	4.66184900
C	-2.65124300	0.98039500	3.36076900
H	-4.45701500	-3.46823000	-3.34616300
H	-2.81735400	1.46090600	5.44432400
C	-4.99184200	-1.62564600	1.66932900
C	-6.28187000	-0.78153300	1.37295100
H	-5.97763900	0.22899400	1.07637400
H	-6.93078600	-0.68971400	2.24901700
H	-6.47450000	-1.89963700	4.23439800
H	-5.18119600	-2.95816000	4.78428200
C	-3.40003700	-2.45219000	-0.29078300
H	-6.60734900	-2.58711400	-2.47887600
H	-4.32291900	-0.43412900	5.99729800
C	-6.95299900	-1.48870200	0.17939000
H	-7.54393500	-0.80577700	-0.44160600
H	-7.63659300	-2.28137100	0.51529900
C	-5.45398200	-2.23672700	4.00540300
C	-5.36312800	-2.83904300	2.58287400
H	-4.55149500	-3.57420000	2.54031300
H	-6.28437000	-3.33716700	2.26407100
C	-1.79337800	2.17275800	3.06728900
C	-0.51117300	2.30583900	3.65347200
C	-2.32649500	3.22848200	2.28221000
C	0.08287900	1.27661400	4.45015600
C	0.25098800	3.51773200	3.44739700
C	-1.54468300	4.42592800	2.06914200
C	1.31634800	1.44149000	5.02376500
H	-0.44949200	0.34249000	4.57252500
C	1.53336600	3.65050400	4.06628600
C	-0.28076700	4.53761200	2.65512800
C	2.05034200	2.64721600	4.84028400
H	1.74748100	0.63518600	5.60937700
H	2.08666600	4.57373200	3.90874500
H	0.29580200	5.44797000	2.50151700
H	3.02440600	2.76153800	5.30909500
C	-2.07482600	-3.56572200	-2.18590400
C	-1.54931200	-2.99616800	-3.37193900
C	-1.50382600	-4.74909700	-1.65367600
C	-2.04527300	-1.77320200	-3.93115000
C	-0.46817000	-3.65785300	-4.06706600
C	-0.38606900	-5.36872600	-2.32941100

C	-1.56110300	-1.27781000	-5.11488900
H	-2.81514000	-1.22720400	-3.39955200
C	-0.00507500	-3.11970400	-5.30962500
C	0.09033300	-4.81710000	-3.52216200
C	-0.54262900	-1.97239900	-5.82910300
H	-1.95396300	-0.34375200	-5.50471100
H	0.78265200	-3.65297800	-5.83798600
H	0.90415500	-5.31363300	-4.04784000
H	-0.18988200	-1.58135800	-6.78003700
C	-4.12252200	4.23035400	0.95564100
H	-5.12173100	4.16908900	0.53239500
C	-3.63705200	3.19021600	1.70484200
H	-4.25950500	2.31975700	1.87568800
C	-3.33467900	5.39337900	0.72636100
H	-3.72667700	6.20329300	0.11778500
C	-2.08462700	5.48587000	1.27544600
H	-1.47131500	6.36750300	1.11067900
C	-1.43204100	-6.54133700	0.00646400
H	-1.83264100	-7.00665200	0.90296100
C	-0.31350500	-7.13033700	-0.64769000
H	0.13229200	-8.03505500	-0.24331200
C	0.18816400	-6.55984200	-1.78542600
H	1.03397900	-7.00562600	-2.30388500
C	-2.00716400	-5.39728500	-0.48069100
H	-2.86198500	-4.96992700	0.02930200
C	5.31767300	-0.44629000	-0.57788800
C	5.01577400	-0.88602700	-2.06727800
H	5.68701600	-0.31354300	-2.71341600
H	5.31728100	-1.93884100	-2.15902400
C	3.63404800	-0.80056500	-2.65539500
C	4.52579900	0.84174600	-0.20779400
H	4.90324400	1.69008000	-0.77758600
H	4.68319900	1.04063400	0.85611400
N	3.06723700	0.79420800	-0.40061200
C	2.34254500	1.69543600	-1.08485500
N	1.00106700	1.67066600	-0.94435100
C	0.08625900	2.56493000	-1.57180700
C	0.23770300	3.94953400	-1.45136100
C	-1.01150600	2.03487500	-2.25301600
C	-0.68953600	4.79827600	-2.04999600
C	-1.93836800	2.90089100	-2.83799200
H	-1.14777900	0.96029900	-2.29245600
C	-1.78084700	4.28173000	-2.75043800
H	-2.51126400	4.94699200	-3.19491700

C	-3.09296500	2.32557400	-3.61508900
C	-0.50985300	6.29061900	-1.96439000
F	-2.72511500	1.99912800	-4.88184700
F	-4.11758900	3.19721000	-3.72108100
F	-3.57318800	1.19841400	-3.04760600
F	0.24800000	6.65171600	-0.90350700
F	-1.69579200	6.93161100	-1.85052500
F	0.09568000	6.78492000	-3.06759600
S	3.10842400	2.72884200	-2.26973100
H	1.05605400	4.35997100	-0.87385500
H	0.54464900	0.84449000	-0.51747500
H	2.55897400	0.25156600	0.31958300
C	3.45440300	0.07414100	-3.72795800
H	4.38054800	0.37465000	-4.22820600
H	3.39140800	1.26308000	-3.04907300
N	-0.49108600	-1.35460400	1.98296600
S	1.04839600	-1.66414000	1.85885600
O	1.89138600	-0.42917500	1.85718000
O	1.46243300	-2.68590400	0.87893300
C	1.34879800	-2.46638100	3.51872300
F	0.97675600	-1.68474300	4.53932200
F	2.65886900	-2.72254900	3.63633600
F	0.67678800	-3.61554700	3.58971300
C	2.54317900	-1.71742300	-2.19354000
H	1.55810900	-1.24159700	-2.18338000
H	2.46288300	-2.54280000	-2.91869700
H	2.71596300	-2.15405800	-1.21060600
C	2.22473000	0.07868900	-4.61579300
H	2.21473500	0.97580000	-5.24216700
H	2.21250800	-0.79623600	-5.27557900
H	1.29437000	0.06145200	-4.04208400
C	6.83187300	-0.12655400	-0.51827100
C	7.75801300	-0.94585600	-1.18873700
C	7.34886100	0.94847100	0.22171100
C	9.12924300	-0.69865500	-1.13467600
H	7.41512800	-1.80277800	-1.75998500
C	8.72176400	1.20004600	0.27856500
H	6.69031300	1.60688700	0.77504800
C	9.62084800	0.38088900	-0.40040600
H	9.81223200	-1.35487200	-1.66774500
H	9.08330500	2.04355400	0.86064200
H	10.68836400	0.57801400	-0.35713900
C	4.99604700	-1.61341900	0.43287100
H	5.33430800	-2.54660500	-0.03538100

H	3.91134400	-1.70458300	0.53942100
C	5.63290600	-1.51749600	1.81876500
C	5.02061900	-0.83842200	2.80367300
H	4.05463700	-0.38964600	2.58441600
C	6.91084200	-2.30377400	2.00427400
H	6.72054700	-3.37332200	1.83358000
H	7.68387700	-2.00373100	1.28893200
H	7.32802700	-2.20290500	3.00856200
C	5.45825400	-0.66439000	4.23128300
H	5.47344200	0.39914100	4.50568000
H	4.73713800	-1.14860300	4.90405900
H	6.44714700	-1.07778900	4.44520400

TS-EF-6SS-5

l imaginary frequency

H = -5393.922697

G = -5394.128248

E(M06-2X-DCM) = -5394.844790

O	-2.09466100	-2.46439900	0.44154400
O	-2.52408700	-0.03493300	1.21021400
P	-1.33928100	-1.03136700	0.67539200
O	-0.77644700	-0.41258300	-0.56850000
C	-5.42243900	-2.71843400	-2.08494600
C	-5.56502900	-2.30096400	-0.76601600
C	-4.46320300	-2.27665200	0.10312400
C	-3.02589800	-3.04336300	-1.71618100
C	-4.16438700	-3.11369600	-2.53708200
C	-3.12259100	-0.25473900	2.44978000
C	-4.09845200	-1.24046000	2.57556800
C	-4.54009200	-1.60371400	3.85712400
C	-4.11957100	-0.89454200	4.97753600
C	-3.26674500	0.19739000	4.80781500
C	-2.74090800	0.53818000	3.55048500
H	-4.04410600	-3.47254200	-3.55504600
H	-2.97977200	0.79754400	5.66629600
C	-4.92776800	-1.97209900	1.52429600
C	-6.23793200	-1.16677100	1.21522800
H	-5.96710600	-0.12580400	1.00385300
H	-6.93552000	-1.16480800	2.05827900
H	-6.51062400	-2.50803400	3.98040400
H	-5.21325100	-3.57396000	4.50690500
C	-3.19751700	-2.57861200	-0.39748800
H	-6.27742200	-2.74494900	-2.75579100
H	-4.46543300	-1.16714200	5.97153600

C	-6.81238900	-1.82060700	-0.05839100
H	-7.39822700	-1.12179100	-0.66641300
H	-7.47853300	-2.65979300	0.18732700
C	-5.46976000	-2.79673700	3.77776000
C	-5.28980900	-3.27148100	2.31711000
H	-4.44650800	-3.96866000	2.25407500
H	-6.17307800	-3.77616800	1.91284700
C	-1.87995500	1.75426300	3.40612200
C	-0.62922800	1.83653000	4.06619000
C	-2.37129200	2.86826900	2.67622300
C	-0.07002600	0.74635500	4.80666000
C	0.13870600	3.06019200	3.99600000
C	-1.57506600	4.07149000	2.58521500
C	1.12817700	0.86847100	5.46004300
H	-0.59726800	-0.19917900	4.81988000
C	1.38351200	3.14637500	4.69472500
C	-0.34750100	4.13596600	3.24990200
C	1.86239400	2.08704000	5.41612400
H	1.53399100	0.01862700	6.00075000
H	1.93969900	4.07962600	4.63955600
H	0.23825900	5.05175100	3.19394500
H	2.80797000	2.16570400	5.94649900
C	-1.70954800	-3.50293200	-2.25887900
C	-1.12300900	-2.82262100	-3.35376400
C	-1.10528000	-4.67919100	-1.74838000
C	-1.66727000	-1.61423600	-3.89827500
C	0.07637600	-3.34969300	-3.96485700
C	0.11451500	-5.17315100	-2.34586200
C	-1.10327600	-0.99966200	-4.98702200
H	-2.54262100	-1.17765800	-3.43310400
C	0.62872600	-2.68464900	-5.10542800
C	0.66606700	-4.50220300	-3.44039000
C	0.05394600	-1.54863400	-5.61092500
H	-1.54233100	-0.08483700	-5.37305800
H	1.51307400	-3.11470600	-5.57146000
H	1.56997500	-4.89492300	-3.90263300
H	0.47492400	-1.06230200	-6.48726600
C	-4.09343500	3.97088200	1.33207900
H	-5.07135100	3.94696000	0.85834200
C	-3.65255100	2.88051500	2.03568800
H	-4.28888000	2.00740000	2.11962200
C	-3.28648500	5.13737200	1.21369000
H	-3.63837800	5.98357800	0.63108300
C	-2.06522200	5.18281200	1.82996800

H	-1.43905900	6.06777200	1.75047700
C	-1.05975600	-6.57395900	-0.20465000
H	-1.50894300	-7.12701500	0.61584400
C	0.15510100	-7.04083700	-0.78127400
H	0.62453300	-7.94105600	-0.39380900
C	0.71962800	-6.35912500	-1.82447900
H	1.64112700	-6.71002100	-2.28351900
C	-1.66730600	-5.43866400	-0.67267600
H	-2.59585800	-5.10532800	-0.22473600
C	5.22924000	0.33557300	-0.19122200
C	5.36960400	0.17412200	-1.74158600
H	5.89302100	1.05294700	-2.12385100
H	6.02037200	-0.69598100	-1.91713600
C	4.15752900	-0.01933400	-2.61221700
C	4.18225400	1.45586300	0.13208100
H	4.52197600	2.39876300	-0.29777100
H	4.13401600	1.57695700	1.21759300
N	2.79868800	1.22572700	-0.30642500
C	2.04131700	2.09798100	-1.00228300
N	0.70567900	1.90993500	-0.98136700
C	-0.27063200	2.73716600	-1.60154900
C	-0.27907000	4.12233000	-1.40770900
C	-1.28550800	2.12661500	-2.34140800
C	-1.28174900	4.89310200	-1.98942500
C	-2.28894900	2.91409300	-2.91117100
H	-1.29520500	1.04749100	-2.44334000
C	-2.29082400	4.29732400	-2.74817800
H	-3.07985800	4.90018400	-3.18149000
C	-3.35161000	2.25539000	-3.75005800
C	-1.27788700	6.38910900	-1.81989800
F	-2.90262700	1.99467200	-5.00623100
F	-4.44797900	3.03047900	-3.88299700
F	-3.74858200	1.07458000	-3.22829900
F	-0.56002500	6.78038700	-0.74379000
F	-2.53225700	6.87684200	-1.66938300
F	-0.74746300	7.01173300	-2.89667400
S	2.77920600	3.31701500	-2.00263000
H	0.47186100	4.59056000	-0.78527600
H	0.31301800	1.02256100	-0.61144200
H	2.29708900	0.59477600	0.33861800
C	3.93075500	0.96184300	-3.59467900
H	4.83357300	1.51575500	-3.87553900
H	3.48999400	1.93066500	-2.85594400
N	-0.36222500	-1.37102400	1.92073800

S	1. 19025200	-1. 52399200	1. 70513100
O	1. 94359300	-0. 25531100	1. 92186300
O	1. 62692700	-2. 29779100	0. 52201700
C	1. 64872300	-2. 59557000	3. 16063900
F	1. 22063000	-2. 08403600	4. 31915200
F	2. 98592500	-2. 69162000	3. 20218400
F	1. 13274500	-3. 81579300	3. 00974900
C	3. 30477000	-1. 24005300	-2. 49837800
H	2. 69719700	-1. 40470500	-3. 38964600
H	3. 95281100	-2. 10840800	-2. 33029800
H	2. 62914700	-1. 21887400	-1. 63526700
C	2. 92333300	0. 80946300	-4. 72290400
H	2. 79474000	1. 76832400	-5. 23381200
H	3. 26685900	0. 07771300	-5. 46377200
H	1. 94160000	0. 48989200	-4. 36471800
C	6. 55663900	0. 88156100	0. 40570400
C	7. 69810800	1. 18581500	-0. 35190800
C	6. 63062400	1. 11769400	1. 79147600
C	8. 85432300	1. 69967600	0. 24143700
H	7. 72133700	1. 00945100	-1. 42109500
C	7. 77950300	1. 63544600	2. 38700600
H	5. 78223200	0. 88876400	2. 42908000
C	8. 90216100	1. 93168100	1. 61356700
H	9. 71914200	1. 91585200	-0. 38027900
H	7. 79417600	1. 80391500	3. 46048000
H	9. 79996100	2. 33353000	2. 07472500
C	4. 82795000	-1. 00922400	0. 49973300
H	3. 78816500	-1. 23104900	0. 26153300
H	4. 83271300	-0. 83192200	1. 58282100
C	5. 64889500	-2. 26228800	0. 21218600
C	4. 99291700	-3. 37622700	-0. 16634100
H	3. 90997800	-3. 30881600	-0. 26530700
C	7. 13205800	-2. 23233900	0. 50494700
H	7. 68668600	-1. 59047300	-0. 18927600
H	7. 31845000	-1. 82333800	1. 50577600
H	7. 58046800	-3. 22739600	0. 46348400
C	5. 54547000	-4. 75179200	-0. 41868800
H	5. 11306500	-5. 47312200	0. 28814300
H	5. 26707900	-5. 10194600	-1. 42216700
H	6. 63364200	-4. 81391600	-0. 33751200

TS-EF-6SS-6

l imaginary frequency

H = -5393. 922994

G = -5394.128062

E(M06-2X-DCM) = -5394.844453

O	-1.90735300	-2.60462000	0.36517700
O	-2.58161500	-0.22464000	1.11400000
P	-1.29179400	-1.11221300	0.63553700
O	-0.72563200	-0.44914900	-0.58451700
C	-5.08924700	-3.13555400	-2.30265100
C	-5.32358100	-2.74542900	-0.98845700
C	-4.26493500	-2.62744900	-0.07473100
C	-2.68922000	-3.23898200	-1.83745100
C	-3.78237700	-3.40618500	-2.70502300
C	-3.20983900	-0.50424400	2.32742500
C	-4.09575300	-1.57572100	2.41172900
C	-4.55182600	-1.98547700	3.67419500
C	-4.24107300	-1.24852600	4.81232300
C	-3.48517700	-0.08256900	4.67939900
C	-2.94480800	0.31261600	3.44453300
H	-3.58783300	-3.74053600	-3.71981500
H	-3.28649900	0.53524400	5.55026200
C	-4.81195800	-2.37547900	1.32718600
C	-6.17781900	-1.69278600	0.96738700
H	-5.99647300	-0.62986800	0.77003100
H	-6.90595300	-1.76089900	1.78135300
H	-6.43417300	-3.06762800	3.71706500
H	-5.06612400	-4.01258600	4.29335000
C	-2.95732200	-2.80850300	-0.52330000
H	-5.91003600	-3.23529800	-3.00840700
H	-4.59832100	-1.55838100	5.79126500
C	-6.63757100	-2.38855100	-0.33029500
H	-7.26173800	-1.74340300	-0.95912900
H	-7.23130000	-3.28808400	-0.11414400
C	-5.36394600	-3.25841600	3.55575900
C	-5.08326800	-3.70683100	2.10274800
H	-4.17727600	-4.32281500	2.07222900
H	-5.89941700	-4.28880700	1.66280000
C	-2.19381600	1.60329000	3.33805000
C	-0.97522200	1.79007000	4.03546900
C	-2.76428400	2.67729800	2.60615100
C	-0.33938100	0.74438700	4.77820000
C	-0.32105300	3.07962700	4.00208600
C	-2.08114300	3.95033500	2.55490200
C	0.82589800	0.96480700	5.46453900
H	-0.77918400	-0.24470000	4.76567500
C	0.89197900	3.26811500	4.73576900

C	-0.88400200	4.11756800	3.25625400
C	1.44701000	2.24555100	5.45568400
H	1.29334800	0.14720400	6.00516100
H	1.36221600	4.24859000	4.70745500
H	-0.38427100	5.08421900	3.22921600
H	2.36805300	2.40155300	6.01143300
C	-1.31547900	-3.56378700	-2.33320100
C	-0.76158200	-2.82091100	-3.40445000
C	-0.61696000	-4.67981800	-1.80816100
C	-1.39802000	-1.66152100	-3.95600000
C	0.49886300	-3.22922000	-3.98260000
C	0.66341100	-5.04935200	-2.36764700
C	-0.86295900	-0.98878600	-5.02485100
H	-2.32061600	-1.30869300	-3.51146500
C	1.01683200	-2.50965100	-5.10614700
C	1.18022000	-4.32321700	-3.44386700
C	0.35438900	-1.42700200	-5.62154100
H	-1.37126000	-0.11270400	-5.41583700
H	1.94749000	-2.85556000	-5.55186500
H	2.13013600	-4.62639200	-3.88062800
H	0.75127400	-0.89913700	-6.48502700
C	-4.54023000	3.63525700	1.22186900
H	-5.49653800	3.52763100	0.71665800
C	-4.02078400	2.57977400	1.92509800
H	-4.57434400	1.64959300	1.97730000
C	-3.84305500	4.87381200	1.14474100
H	-4.25529800	5.69326100	0.56345700
C	-2.65077500	5.02329700	1.80006300
H	-2.10757600	5.96342700	1.75145800
C	-0.43762800	-6.57219200	-0.27154400
H	-0.85737600	-7.17219500	0.53135200
C	0.83544300	-6.91413500	-0.80876100
H	1.37785300	-7.76658300	-0.40879200
C	1.36443600	-6.17390900	-1.83048200
H	2.33005500	-6.43052400	-2.26023400
C	-1.13749200	-5.49832300	-0.75526500
H	-2.10841900	-5.26040500	-0.33747200
C	5.16865100	0.62260700	-0.09246700
C	5.37363400	0.67537700	-1.64339100
H	5.77404200	1.65924400	-1.89920700
H	6.14478300	-0.06750700	-1.89404400
C	4.23043900	0.40508400	-2.57614100
C	4.05870300	1.65494900	0.31320800
H	4.35346900	2.64968600	-0.02342400

H	3.99024700	1.67018500	1.40443200
N	2.69775500	1.38718000	-0.17112700
C	1.91225500	2.24899300	-0.84875700
N	0.59159400	1.97788200	-0.88530200
C	-0.41405500	2.75259200	-1.52660900
C	-0.53341400	4.12775300	-1.30116100
C	-1.34637500	2.09005200	-2.32809500
C	-1.56245900	4.83847600	-1.91297900
C	-2.37809700	2.81678900	-2.92689100
H	-1.27171500	1.01621200	-2.45609000
C	-2.48908700	4.19142800	-2.73257100
H	-3.29908200	4.74704400	-3.18978100
C	-3.34799200	2.10458300	-3.83180000
C	-1.67486800	6.32662200	-1.71389400
F	-2.82365600	1.91585200	-5.07175200
F	-4.49356700	2.79796700	-3.99635900
F	-3.67566000	0.88198400	-3.36068700
F	-1.03060500	6.74479000	-0.60189100
F	-2.96613900	6.71943300	-1.60644200
F	-1.14846100	7.00942500	-2.75585200
S	2.60244200	3.56768400	-1.75168000
H	0.15236700	4.63283500	-0.63422000
H	0.24590500	1.05246300	-0.56280000
H	2.21705700	0.69948200	0.42879300
C	3.91787400	1.41721000	-3.50098500
H	4.76259700	2.08012300	-3.72179400
H	3.38273300	2.28779000	-2.70933000
N	-0.35171300	-1.35375200	1.93028000
S	1.20991900	-1.49847000	1.77512300
O	1.94158200	-0.22073900	2.01029100
O	1.69462500	-2.28363000	0.62168200
C	1.62024500	-2.54211800	3.26568600
F	1.14159700	-2.01871900	4.39859400
F	2.95922600	-2.62142700	3.36914000
F	1.12869300	-3.77159900	3.11461000
C	3.51952200	-0.91140500	-2.57389800
H	3.11070300	-1.14923600	-3.55864300
H	4.20572400	-1.70436100	-2.26000300
H	2.68003200	-0.93623900	-1.86751500
C	2.95775400	1.22462400	-4.66234400
H	2.71435600	2.19428300	-5.10670800
H	3.40498400	0.60058400	-5.44570100
H	2.02042600	0.75513200	-4.35292300
C	6.44155100	1.13955900	0.63296400

C	7.54770700	1.70197000	-0.02311000
C	6.48579800	1.09625400	2.03841700
C	8.64743500	2.19009000	0.68783400
H	7.58651200	1.75598300	-1.10501700
C	7.57796100	1.58681800	2.75124200
H	5.65803300	0.66938800	2.59599200
C	8.66913200	2.13837000	2.07910200
H	9.48782600	2.61176600	0.14274300
H	7.57368800	1.53361600	3.83662400
H	9.52298100	2.51940700	2.63228300
C	4.77875200	-0.79750700	0.40544800
H	3.77992700	-1.03487600	0.03193000
H	4.62115000	-0.74775100	1.49009400
C	5.66000900	-2.01115700	0.12510200
C	6.94304600	-1.95293700	-0.27229500
H	7.40328600	-0.97512900	-0.38856400
C	4.92748900	-3.30507300	0.41019600
H	4.54808600	-3.30812700	1.43928200
H	4.03990600	-3.41183500	-0.22478800
H	5.55498100	-4.18895400	0.28070400
C	7.88831400	-3.09337100	-0.54063900
H	8.32125800	-3.01128200	-1.54715200
H	8.73345000	-3.06797200	0.16129700
H	7.42093700	-4.07746600	-0.46142100

TS-EF-6SR

l imaginary frequency

H = -5393.923070

G = -5394.132250

E(M06-2X-DCM) = -5394.853687

O	-0.69430600	-2.66695000	-0.52020900
O	-2.70872300	-1.12201000	0.02990600
P	-1.06972300	-1.15450600	-0.00827600
O	-0.63728800	-0.09337300	-0.96971300
C	-1.84487900	-3.60173700	-4.43431600
C	-2.73875400	-3.73691300	-3.37703600
C	-2.32108100	-3.50283100	-2.05931800
C	-0.09408200	-2.91031500	-2.86509200
C	-0.52889300	-3.22541700	-4.16483700
C	-3.41598700	-2.04673300	0.79835100
C	-3.62089700	-3.33773500	0.30748100
C	-4.19972500	-4.30304700	1.14783300
C	-4.66640100	-3.96190400	2.41213200
C	-4.56282600	-2.63780000	2.83503300

C	-3.93377500	-1.65721100	2.05055600
H	0.18652000	-3.14868400	-4.97831800
H	-4.95918100	-2.34590900	3.80314600
C	-3.40879000	-3.93510600	-1.08353600
C	-4.67564000	-3.74356500	-1.98483000
H	-4.96788300	-2.68718700	-1.95795400
H	-5.52919800	-4.33546400	-1.63974500
H	-5.21713500	-5.93327600	0.14325200
H	-3.87364300	-6.45941600	1.15199600
C	-1.03464400	-3.02542400	-1.82304700
H	-2.15823800	-3.79389200	-5.45751800
H	-5.11675700	-4.70973700	3.05992000
C	-4.20374400	-4.11623300	-3.40823500
H	-4.75906600	-3.58513400	-4.19002100
H	-4.33462100	-5.18963500	-3.60486800
C	-4.20693200	-5.66042100	0.47991200
C	-3.25312100	-5.44896300	-0.71377300
H	-2.21917400	-5.62682700	-0.39681300
H	-3.46108300	-6.10930900	-1.56141500
C	-3.90987100	-0.24814700	2.55818900
C	-3.15920800	0.08117600	3.71265300
C	-4.74395200	0.72499300	1.95206100
C	-2.27945600	-0.84958700	4.35181400
C	-3.25824000	1.40897200	4.27771700
C	-4.80959600	2.05842600	2.50794900
C	-1.57193800	-0.50573400	5.47278800
H	-2.14586000	-1.82808700	3.91021800
C	-2.51490400	1.72168800	5.45956100
C	-4.07275800	2.36134900	3.65725700
C	-1.69853900	0.79208100	6.04434500
H	-0.88742900	-1.22277300	5.91556500
H	-2.61202300	2.72022700	5.88008900
H	-4.14869600	3.35801100	4.08900600
H	-1.13288100	1.04341600	6.93749000
C	1.33186600	-2.51183100	-2.64790400
C	1.84175800	-1.34459700	-3.27039800
C	2.19740300	-3.35209100	-1.90283300
C	1.01838700	-0.43032900	-4.00652800
C	3.25115300	-1.03595600	-3.16791200
C	3.59375500	-3.00276700	-1.76944600
C	1.55443200	0.66142100	-4.64127300
H	-0.05023500	-0.60449800	-4.04756400
C	3.77033200	0.11163200	-3.84856800
C	4.08506900	-1.86297400	-2.41112800

C	2.95118400	0.93492200	-4.57405800
H	0.90429200	1.32649200	-5.20425000
H	4.83831000	0.30723900	-3.77920700
H	5.13991100	-1.61131400	-2.32038900
H	3.35926900	1.79737600	-5.09443600
C	-6.37764000	1.40142400	0.25975300
H	-7.00284000	1.15357000	-0.59395400
C	-5.57369100	0.44120800	0.81883200
H	-5.57018800	-0.56233900	0.40870200
C	-6.41286400	2.72160600	0.79269600
H	-7.05396400	3.47054600	0.33581800
C	-5.65263900	3.03397100	1.88748100
H	-5.68653400	4.03208500	2.31914700
C	2.62150100	-5.35186600	-0.56298700
H	2.25839000	-6.26584000	-0.10068600
C	3.98870900	-4.98640300	-0.41125300
H	4.65460000	-5.61846900	0.16987900
C	4.45775800	-3.84630000	-1.00406600
H	5.50188900	-3.55863100	-0.90730400
C	1.76107700	-4.56715600	-1.28471800
H	0.72660800	-4.87008000	-1.39468200
C	-1.36135900	3.50400200	-1.78236100
C	-1.61179500	3.27470100	-0.26117900
H	-2.55828800	3.77182200	0.00624300
H	-1.77491200	2.20738500	-0.10795200
C	-0.60652900	3.70018500	0.78475800
C	0.14941800	3.24216100	-2.10395200
H	0.71889000	4.16749800	-2.03331600
H	0.25413300	2.87708400	-3.12877200
N	0.79352800	2.26275100	-1.22701700
C	2.02179300	2.39031400	-0.70246700
N	2.60286500	1.29474400	-0.18441200
C	3.93978600	1.23338200	0.31552500
C	5.00222200	1.37364300	-0.57467300
C	4.17452100	0.93830200	1.66002300
C	6.31176700	1.22087100	-0.12010500
C	5.49119000	0.80190400	2.10383100
H	3.33981000	0.80547800	2.34054200
C	6.56434600	0.93947400	1.22097900
H	7.58155800	0.82296900	1.57394000
C	5.75336800	0.44116300	3.54439700
C	7.42800600	1.33457600	-1.12204900
F	5.70662900	-0.89424300	3.73939900
F	4.84479900	0.99745800	4.37104700

F	6.97766800	0.85603300	3.94529600
F	7.22878200	0.48807800	-2.16807700
F	8.63025600	1.03902300	-0.59062800
F	7.50852800	2.57639200	-1.64736900
S	2.78030600	3.95369500	-0.55563500
H	4.79854000	1.57125600	-1.62098100
H	2.08807800	0.40591700	-0.12231000
H	0.35407500	1.32428500	-1.20394700
C	0.15364600	4.87605000	0.73621900
H	-0.16479200	5.60185700	-0.01115100
H	1.25782700	4.45332800	0.12506700
N	-0.60923600	-1.09546300	1.54119200
S	0.90779200	-1.16759400	1.99352500
O	1.19858700	-0.21647500	3.07786200
O	1.88179000	-1.21821400	0.87037800
C	1.05562200	-2.85268200	2.79034100
F	0.75001400	-3.81446900	1.91655200
F	0.22433700	-2.94535800	3.84099300
F	2.30780800	-3.03209000	3.22089100
C	-2.25520600	2.55865700	-2.62694200
C	-3.29336500	1.78569300	-2.09170100
C	-2.06828200	2.50663000	-4.02077600
C	-4.09773700	0.98705100	-2.90898800
H	-3.50353100	1.78290800	-1.03003200
C	-2.86601600	1.70980600	-4.83946100
H	-1.29496000	3.10802700	-4.49153800
C	-3.88959500	0.94013500	-4.28481700
H	-4.88762400	0.39901300	-2.45079900
H	-2.68863900	1.69612100	-5.91177100
H	-4.51387000	0.31560100	-4.91798600
C	-1.66721400	4.98703700	-2.23001100
H	-0.94346500	5.64923900	-1.74628300
H	-1.45141700	5.05060400	-3.30425700
C	-3.06538600	5.53235600	-1.97191900
C	-3.27717900	6.29703600	-0.88577500
H	-2.42325300	6.48781200	-0.23278400
C	-0.51677100	2.77931900	1.95910000
H	0.32589400	2.98613200	2.61940600
H	-1.43792100	2.88782300	2.55400300
H	-0.48678000	1.72699300	1.66206600
C	-4.12954400	5.22393000	-3.00064100
H	-5.02506200	5.83545400	-2.86767300
H	-3.74707200	5.40890100	-4.01248400
H	-4.43301600	4.17226000	-2.97061700

C	0.76674100	5.52691600	1.97601100
H	1.43749100	6.33554100	1.66979700
H	-0.01018500	5.95823300	2.61780000
H	1.35272400	4.82535300	2.57451700
C	-4.55147300	6.94762300	-0.42544500
H	-4.41425700	8.03041700	-0.30265900
H	-5.38903400	6.79051800	-1.10916100
H	-4.85115700	6.55819900	0.55746200

TS-EF-6SR-1

l imaginary frequency

H = -5393.921813

G = -5394.131185

E(M06-2X-DCM) = -5394.850838

O	-1.31904700	-2.66315400	-0.73512100
O	-2.99436500	-0.81211000	-0.03832500
P	-1.39613400	-1.14087900	-0.13139000
O	-0.81897100	-0.11379900	-1.05842700
C	-2.65282700	-3.07861800	-4.68001600
C	-3.55317900	-3.10372600	-3.61969100
C	-3.09497900	-3.05528600	-2.29464300
C	-0.79540400	-2.87162300	-3.09759300
C	-1.28620500	-3.00022700	-4.40832300
C	-3.85852300	-1.63465600	0.68373700
C	-4.33074800	-2.81081800	0.09988800
C	-5.09155700	-3.69875000	0.87729500
C	-5.46672900	-3.36777200	2.17466000
C	-5.07731800	-2.13606200	2.69829200
C	-4.25900100	-1.24910500	1.97837500
H	-0.57201400	-3.01459500	-5.22646200
H	-5.39064700	-1.85010800	3.69792500
C	-4.24890900	-3.32864100	-1.33582700
C	-5.44979200	-2.81545600	-2.20044800
H	-5.52178100	-1.72681000	-2.09148200
H	-6.40587400	-3.24525700	-1.88585500
H	-6.42838300	-4.99889500	-0.23030100
H	-5.22207600	-5.86960100	0.71093400
C	-1.73730300	-2.86490700	-2.05027300
H	-3.00203700	-3.12818700	-5.70839500
H	-6.06161100	-4.05269900	2.77362500
C	-5.06513400	-3.17076600	-3.65437500
H	-5.49949300	-2.48104700	-4.38727100
H	-5.41411100	-4.17693500	-3.92578500
C	-5.38306100	-4.96847100	0.10827400

C	-4.40781300	-4.86645000	-1.08292300
H	-3.43234000	-5.27691800	-0.79799700
H	-4.74880000	-5.40309800	-1.97371100
C	-3.90032500	0.06283300	2.60483900
C	-3.12682600	0.08805500	3.79182800
C	-4.42972500	1.26754400	2.07600500
C	-2.50894000	-1.08245500	4.33839000
C	-2.91962500	1.33965000	4.48563100
C	-4.18404200	2.51727900	2.76124000
C	-1.77560700	-1.02782700	5.49395600
H	-2.59248600	-2.01715100	3.79910500
C	-2.16442700	1.34911800	5.70063800
C	-3.45249200	2.51703900	3.95271900
C	-1.61200900	0.19971500	6.19614300
H	-1.29388700	-1.92672600	5.86724600
H	-2.03320000	2.29720200	6.21757300
H	-3.29850100	3.45654900	4.48105400
H	-1.03264600	0.22076500	7.11522200
C	0.67932800	-2.78408800	-2.85978500
C	1.41881500	-1.68806200	-3.36959100
C	1.34739100	-3.83943100	-2.18894800
C	0.80829800	-0.58470100	-4.05146300
C	2.85571000	-1.65592400	-3.20589100
C	2.77905500	-3.77646600	-2.00427200
C	1.55881000	0.43853300	-4.57204300
H	-0.27078700	-0.56381800	-4.14688300
C	3.60156400	-0.56548600	-3.75741200
C	3.49300700	-2.69161500	-2.51894100
C	2.97685900	0.45011900	-4.43078400
H	1.06769100	1.25305600	-5.09848200
H	4.68255000	-0.56755800	-3.63333400
H	4.57302800	-2.65810900	-2.39048700
H	3.55525800	1.26533100	-4.85753200
C	-5.72082500	2.49646600	0.39981100
H	-6.31789800	2.49955900	-0.50773400
C	-5.23311500	1.31364400	0.89103800
H	-5.45874500	0.38730500	0.37590100
C	-5.45458700	3.72612100	1.06618300
H	-5.85211900	4.65395400	0.66358600
C	-4.71366100	3.72995600	2.21720600
H	-4.51883000	4.65882200	2.74915100
C	1.34647600	-6.00380200	-1.05308300
H	0.80429200	-6.87317700	-0.69085300
C	2.75281600	-5.92171400	-0.84988900

H	3.27018500	-6.72268600	-0.32894200
C	3.44554400	-4.83889300	-1.31816100
H	4.52158300	-4.76549400	-1.17983800
C	0.67108800	-5.00235000	-1.69982000
H	-0.39837400	-5.09018600	-1.85149500
C	-0.68597400	3.92077300	-1.50238200
C	-1.04388700	3.62260600	-0.00314700
H	-1.73991900	4.39986900	0.33389000
H	-1.60715300	2.68894800	0.02421700
C	0.03939300	3.53426700	1.04904900
C	0.37798000	2.86462500	-2.03432300
H	1.18632500	3.39188500	-2.54289700
H	-0.10393100	2.21266600	-2.76308500
N	0.98376200	1.94715200	-1.06121000
C	2.26775500	1.93526000	-0.67857400
N	2.76634200	0.78725200	-0.18748400
C	4.09403300	0.58008400	0.28646800
C	5.18064600	0.78475700	-0.56467700
C	4.28859900	0.08474600	1.57817300
C	6.47150600	0.51417600	-0.11360100
C	5.58774400	-0.18367600	2.01450900
H	3.43602800	-0.09115300	2.22682900
C	6.68317700	0.03202000	1.17787300
H	7.68682800	-0.18136200	1.52503700
C	5.80202000	-0.76591600	3.38929100
C	7.63454900	0.77064700	-1.03501800
F	5.69066800	-2.11193600	3.37998000
F	4.90100800	-0.29652500	4.27531400
F	7.03427900	-0.47442000	3.86537200
F	7.32639400	0.45630900	-2.31647800
F	8.72125500	0.04925000	-0.68980200
F	8.00110800	2.07135900	-1.03040200
S	3.19061400	3.41633000	-0.66462600
H	5.01225000	1.12349100	-1.57983900
H	2.15346200	-0.03895800	-0.09214600
H	0.44227500	1.06781200	-0.95904000
C	1.01812000	4.50963200	1.20224100
H	0.81934000	5.45092800	0.69122200
H	1.96444700	4.02969500	0.26941700
N	-0.87833600	-1.25232900	1.39526400
S	0.62692200	-1.54747600	1.78844400
O	1.06977600	-0.73209500	2.92963600
O	1.56221000	-1.62195600	0.62995800
C	0.58158600	-3.29800700	2.44369100

F	0.13134600	-4.13677500	1.50897200
F	-0.22427700	-3.36825400	3.51311000
F	1.81319400	-3.66585200	2.80949000
C	-1.97577400	3.72361700	-2.34478200
C	-2.63245100	2.47886000	-2.32597600
C	-2.50014000	4.71855800	-3.18223700
C	-3.77088300	2.24998000	-3.09681700
H	-2.24636700	1.65774400	-1.72866100
C	-3.64099900	4.48982200	-3.95695100
H	-2.03611600	5.69631300	-3.23098100
C	-4.28503800	3.25555600	-3.91708700
H	-4.24753400	1.27419700	-3.05737000
H	-4.02025100	5.28533900	-4.59340900
H	-5.17083800	3.07671800	-4.52100100
C	-0.04199000	5.32366400	-1.73760200
H	1.00186300	5.25724000	-1.41466300
H	0.04161600	5.45417300	-2.82797300
C	-0.59779800	6.62091500	-1.15783300
C	-1.84873700	6.78977800	-0.69765600
H	-2.53323600	5.94669700	-0.75192000
C	-0.06383900	2.38310600	2.00076800
H	0.87925300	2.12740700	2.48792800
H	-0.76764600	2.66011700	2.80175200
H	-0.47365900	1.48469700	1.53682900
C	0.43134400	7.73161100	-1.20990100
H	0.03873300	8.70015300	-0.89548400
H	1.30019800	7.50143900	-0.57717500
H	0.81952000	7.84650000	-2.23126100
C	1.87853200	4.65208000	2.44988900
H	2.70808900	5.33986000	2.25788600
H	1.29359000	5.05974600	3.28358400
H	2.30837900	3.70157900	2.77698300
C	-2.47340300	8.03199600	-0.12322100
H	-3.33327400	8.34740700	-0.72987900
H	-2.86300600	7.83541100	0.88478900
H	-1.78663800	8.87869100	-0.05276700

TS-EF-6SR-2

l imaginary frequency

H = -5393.919749

G = -5394.126859

E(M06-2X-DCM) = -5394.845115

0	-0.96641300	-2.99280800	0.28148800
0	-2.47773000	-0.93142200	0.68468000

P	-0.90675200	-1.37716300	0.54573600
O	-0.30507100	-0.62117600	-0.60285300
C	-3.45913900	-4.69074300	-2.62151400
C	-3.94248400	-4.39371600	-1.35170400
C	-3.09733500	-3.85825300	-0.36843200
C	-1.25245100	-3.85923800	-1.96668200
C	-2.11950900	-4.43801100	-2.90992600
C	-3.18146300	-1.31322200	1.83012800
C	-3.60116900	-2.63258700	1.98287000
C	-4.03608200	-3.06610300	3.24481100
C	-4.19856200	-2.15872800	4.28688900
C	-3.96231700	-0.80290900	4.04681900
C	-3.44796800	-0.34950500	2.82198200
H	-1.72382900	-4.67739900	-3.89266800
H	-4.16236800	-0.07151000	4.82469500
C	-3.83630500	-3.74133800	0.96029900
C	-5.31683000	-3.65959600	0.44072600
H	-5.53137100	-2.62181300	0.16038000
H	-6.04336800	-3.95513400	1.20353100
H	-5.34008900	-4.80390700	3.29863800
H	-3.78638600	-5.06378700	4.08233400
C	-1.77592000	-3.55559600	-0.69535300
H	-4.11265200	-5.11075800	-3.38194100
H	-4.53617200	-2.48882900	5.26617000
C	-5.34840900	-4.54763700	-0.81863900
H	-6.11168600	-4.23494600	-1.54029300
H	-5.56331800	-5.59554000	-0.56472200
C	-4.26962700	-4.56378300	3.23497000
C	-3.67243500	-4.99794100	1.87403400
H	-2.60446100	-5.21557700	1.98717300
H	-4.15470700	-5.88687200	1.45433600
C	-3.31996300	1.11977900	2.55669100
C	-2.34393500	1.90528600	3.21245400
C	-4.26461700	1.73464200	1.69432200
C	-1.36328600	1.34060200	4.08793400
C	-2.30864000	3.33464000	2.99376400
C	-4.20805200	3.16197600	1.47397900
C	-0.43243300	2.12741700	4.71441700
H	-1.34911900	0.26795900	4.22867000
C	-1.32360600	4.11955800	3.67147800
C	-3.23361400	3.92199200	2.12743000
C	-0.41442400	3.53679900	4.51222900
H	0.31131000	1.66836500	5.35826300
H	-1.31685600	5.19397100	3.50186800

H	-3.19173800	4.99418600	1.95186300
H	0.32929600	4.14411200	5.02180300
C	0.17270000	-3.62897700	-2.36066200
C	0.46904600	-2.69960600	-3.38738300
C	1.20446800	-4.42080700	-1.79996500
C	-0.51689200	-1.82444800	-3.94979600
C	1.81710800	-2.60561400	-3.89974700
C	2.55629600	-4.28596600	-2.29340600
C	-0.21106800	-0.95843200	-4.96844100
H	-1.52234700	-1.83991300	-3.54652300
C	2.08997700	-1.70761200	-4.98052500
C	2.82276200	-3.39642300	-3.33788100
C	1.10774900	-0.90980600	-5.50586000
H	-0.97758400	-0.29865400	-5.36298200
H	3.10079900	-1.68192200	-5.38309400
H	3.83684000	-3.32519400	-3.72737000
H	1.32691000	-0.24080800	-6.33443100
C	-6.20799700	1.63379200	0.21072700
H	-6.99054000	1.05441600	-0.27225000
C	-5.31019100	1.00878400	1.03656900
H	-5.39421500	-0.05817700	1.20708200
C	-6.13022000	3.03589300	-0.02064500
H	-6.84717500	3.51435600	-0.68257300
C	-5.15881800	3.77514300	0.59861000
H	-5.08707200	4.84612400	0.43066000
C	1.98717100	-6.14211300	-0.25298300
H	1.77925600	-6.86296400	0.53291000
C	3.32019200	-5.99106200	-0.72954600
H	4.11525500	-6.59827300	-0.30480100
C	3.59202400	-5.09051500	-1.72346100
H	4.60366500	-4.97056100	-2.10435800
C	0.96813100	-5.38809100	-0.77165200
H	-0.04023500	-5.51920700	-0.39772100
C	5.30319700	1.71311800	0.00843100
C	5.41828700	2.27740300	-1.45264800
H	5.40478100	3.37137400	-1.39927700
H	6.41378200	2.00670200	-1.83326600
C	4.44028400	1.85043300	-2.50589400
C	3.92608600	2.11447000	0.61540400
H	3.90342900	3.20225800	0.69426300
H	3.84233200	1.70670200	1.62489900
N	2.70460000	1.70475900	-0.10162200
C	1.74189800	2.55440200	-0.55035300
N	0.51284600	2.02934900	-0.71565300

C	-0.61471400	2.63519600	-1.33835300
C	-1.04171300	3.93127700	-1.03490100
C	-1.34659700	1.85046700	-2.23569900
C	-2.16541800	4.45185300	-1.67641500
C	-2.48041100	2.38034500	-2.85193300
H	-1.03860100	0.82836500	-2.42438600
C	-2.89102600	3.68593100	-2.58859200
H	-3.77663300	4.09005300	-3.06315100
C	-3.22926200	1.54408400	-3.85531600
C	-2.57334000	5.87622400	-1.40922500
F	-2.64511500	1.60285200	-5.08305900
F	-4.50306700	1.95816100	-4.01305900
F	-3.26120500	0.24025900	-3.50753900
F	-2.26212000	6.26725700	-0.15153100
F	-3.90424300	6.06099900	-1.57071300
F	-1.95571000	6.73786200	-2.24918100
S	2.13563500	4.17935300	-1.00542100
H	-0.51925900	4.52106600	-0.29529900
H	0.35880600	1.01921600	-0.51781100
H	2.33958800	0.81835400	0.26036600
C	3.83909500	2.89146600	-3.25172600
H	4.47645100	3.78225400	-3.31907100
H	3.13121200	3.37652400	-2.34954200
N	-0.25177100	-1.25468300	2.01804500
S	1.31320100	-1.30496400	2.22187500
O	1.96485900	0.03120500	2.10681100
O	2.02663500	-2.40979100	1.55632800
C	1.41068600	-1.72009700	4.03709300
F	0.79273300	-0.81056200	4.80272200
F	2.70363800	-1.75700200	4.38735700
F	0.86664600	-2.91609300	4.26731900
C	5.64043700	0.21147100	0.02923800
C	6.85249500	-0.23376900	-0.53264700
C	4.79554600	-0.75484500	0.58972600
C	7.19529200	-1.58416300	-0.54599100
H	7.55438000	0.47745500	-0.96218500
C	5.12840000	-2.11382000	0.56710300
H	3.86478600	-0.47822600	1.06810200
C	6.32832200	-2.53448100	-0.00107200
H	8.14099400	-1.89245300	-0.98490000
H	4.42407400	-2.82315700	0.98896600
H	6.58776100	-3.58945700	-0.01976900
C	6.37999300	2.52301600	0.83438200
H	6.21313600	3.58681400	0.62495800

H	7.36629300	2.27515500	0.42027300
C	4.16777200	0.41628800	-2.79292500
H	3.29030600	0.26990900	-3.42350100
H	5.03909700	0.03063800	-3.34909900
H	4.09220200	-0.19889400	-1.89627700
C	6.41331800	2.33604200	2.34404100
C	5.95096300	3.32476200	3.12929100
H	5.55201700	4.21201600	2.63402200
C	7.03369000	1.06149900	2.86851200
H	6.39389900	0.19060200	2.68899700
H	7.98384100	0.85725800	2.35840300
H	7.23479100	1.11053700	3.94100600
C	2.98317000	2.65712900	-4.48690500
H	2.50666100	3.59549600	-4.78487900
H	3.58846500	2.30510000	-5.33044700
H	2.18970200	1.92496600	-4.31269200
C	5.89492900	3.38552900	4.62919100
H	6.32333000	2.50612500	5.11580100
H	6.42569200	4.27192200	5.00227600
H	4.85511100	3.47829200	4.97095600

TS-EF-6SR-3

l imaginary frequency

H = -5393.918340

G = -5394.124596

E(M06-2X-DCM) = -5394.843634

O	1.40870300	-2.84842100	-0.34905700
O	2.58706900	-0.60404100	-0.86051100
P	1.11081600	-1.25180800	-0.56609900
O	0.53923600	-0.57645700	0.64381700
C	4.30978300	-4.17976800	2.35864700
C	4.66229100	-3.79933200	1.06808800
C	3.68451300	-3.39770400	0.14568700
C	1.96328200	-3.70943200	1.84813500
C	2.96591900	-4.15309500	2.72763600
C	3.22707500	-0.90143800	-2.06524300
C	3.83580700	-2.14188500	-2.23971500
C	4.23430900	-2.52967800	-3.52826100
C	4.16259500	-1.63394000	-4.59035000
C	3.72344100	-0.33024400	-4.34829700
C	3.24436600	0.06533200	-3.08946200
H	2.67265200	-4.46912500	3.72453200
H	3.73352000	0.40270500	-5.14997400
C	4.31126500	-3.18016700	-1.22738000

C	5. 78971100	-2. 86336800	-0. 80401900
H	5. 85626000	-1. 80270300	-0. 53534700
H	6. 50378000	-3. 04751300	-1. 61241100
H	5. 79783400	-4. 03230400	-3. 65899600
H	4. 25793900	-4. 55857800	-4. 32819400
C	2. 35603500	-3. 30363900	0. 55831500
H	5. 06653000	-4. 49614800	3. 07210400
H	4. 47153100	-1. 92890200	-5. 59011400
C	6. 03949600	-3. 72754900	0. 44836000
H	6. 78480400	-3. 29147900	1. 12332300
H	6. 40522400	-4. 72846700	0. 17795600
C	4. 70929600	-3. 96870100	-3. 52203100
C	4. 28647000	-4. 46442400	-2. 11821200
H	3. 26132400	-4. 85021500	-2. 15236500
H	4. 93147800	-5. 25793900	-1. 72695200
C	2. 88774800	1. 49855200	-2. 83770200
C	1. 75180000	2. 08973200	-3. 43840500
C	3. 76879000	2. 28809400	-2. 05367700
C	0. 82528400	1. 34465900	-4. 23490900
C	1. 48959100	3. 49883100	-3. 24265700
C	3. 48553800	3. 69129200	-1. 85430800
C	-0. 26114400	1. 94757400	-4. 81269200
H	0. 97939900	0. 27986000	-4. 35161400
C	0. 34692000	4. 08927000	-3. 86828300
C	2. 35447400	4. 25700300	-2. 45009800
C	-0. 50166000	3. 33991000	-4. 63708600
H	-0. 95778100	1. 35272300	-5. 39515600
H	0. 17107200	5. 15226200	-3. 71842300
H	2. 14595200	5. 31289100	-2. 29389500
H	-1. 36612300	3. 80033900	-5. 10867300
C	0. 54055900	-3. 73141100	2. 31081200
C	0. 13664000	-2. 88909100	3. 37461900
C	-0. 36716700	-4. 67263200	1. 76589200
C	0. 99188600	-1. 88625300	3. 93694600
C	-1. 19097400	-3. 02487400	3. 92991800
C	-1. 70419700	-4. 77076200	2. 30567700
C	0. 59055900	-1. 11226800	4. 99578500
H	1. 97266000	-1. 73125400	3. 50389400
C	-1. 56624600	-2. 20915300	5. 04447200
C	-2. 07532700	-3. 95504800	3. 37784800
C	-0. 70151400	-1. 28601600	5. 57095300
H	1. 25950400	-0. 35518800	5. 39314900
H	-2. 55634600	-2. 35076000	5. 47349300
H	-3. 07388700	-4. 05598000	3. 79957700

H	-0.99430500	-0.68425600	6.42778100
C	5.79665500	2.55915000	-0.71117600
H	6.69707800	2.13393300	-0.27554000
C	4.96441600	1.76814900	-1.45978900
H	5.21713500	0.72612800	-1.61745400
C	5.49784600	3.93441100	-0.49966900
H	6.16579300	4.54651100	0.10051400
C	4.37526500	4.48111200	-1.06029800
H	4.13662700	5.53007200	-0.91053800
C	-0.91105700	-6.47728500	0.21115100
H	-0.61444700	-7.14448200	-0.59363800
C	-2.23333900	-6.55428000	0.73274300
H	-2.93359600	-7.27587500	0.32045900
C	-2.61343500	-5.72552100	1.75263000
H	-3.61756700	-5.77880400	2.16712800
C	-0.01204600	-5.57271300	0.71103800
H	0.99132300	-5.53290400	0.30398800
C	-5.46607200	1.35268300	0.29486200
C	-5.53024200	1.63890700	1.83325200
H	-5.61936100	2.72179100	1.97332000
H	-6.46707100	1.21289100	2.21856800
C	-4.43884300	1.14252700	2.73657200
C	-4.15383000	1.95480100	-0.28739300
H	-4.20615400	3.03744500	-0.16671500
H	-4.10283300	1.73519000	-1.35652600
N	-2.86501000	1.52137300	0.28497700
C	-1.94413300	2.35978600	0.82398300
N	-0.66975500	1.92796600	0.87242800
C	0.43334500	2.61329700	1.46086200
C	0.72913100	3.94126900	1.14134300
C	1.26940500	1.89637000	2.32042300
C	1.83085500	4.56145400	1.72819100
C	2.38082400	2.52673100	2.88323000
H	1.06296300	0.85106100	2.51831400
C	2.66247900	3.86223900	2.60313100
H	3.52996600	4.34352400	3.03717000
C	3.24917500	1.75939200	3.84458000
C	2.09665100	6.01559300	1.44406600
F	2.69200000	1.71007000	5.08464700
F	4.46767600	2.31960900	3.98904400
F	3.43069300	0.48002400	3.45370300
F	1.73514300	6.36039900	0.18493200
F	3.40339100	6.33016500	1.58828400
F	1.40436500	6.82201100	2.28066900

S	-2.43083900	3.86218300	1.55143200
H	0.11998400	4.48008100	0.42812600
H	-0.43004300	0.95933400	0.58458100
H	-2.46644900	0.72456100	-0.23150600
C	-3.88949700	2.09617700	3.61641300
H	-4.58602500	2.90977700	3.85351200
H	-3.27595700	2.79756700	2.75135000
N	0.28943900	-1.21929800	-1.96065200
S	-1.28416000	-1.32406800	-1.95556400
O	-1.95702300	0.00973200	-1.92272700
O	-1.88564900	-2.34689500	-1.08327300
C	-1.59851800	-1.94701700	-3.68455600
F	-1.10486100	-1.13079100	-4.62371200
F	-2.92917000	-2.03417100	-3.86040700
F	-1.06604600	-3.15857400	-3.84466800
C	-5.71800400	-0.13498400	-0.01120200
C	-6.81139900	-0.79386900	0.58524700
C	-4.94520300	-0.86548200	-0.92026800
C	-7.10558300	-2.12456900	0.29807900
H	-7.46407400	-0.26612000	1.27654800
C	-5.23017400	-2.20560700	-1.20398100
H	-4.09951900	-0.41593000	-1.42445500
C	-6.30907600	-2.84176200	-0.59811300
H	-7.95795800	-2.60042400	0.77651100
H	-4.58522100	-2.73947900	-1.89316000
H	-6.52885900	-3.88309500	-0.81680600
C	-6.65269200	2.19724500	-0.32676800
H	-6.55934300	3.22538300	0.04886700
H	-7.58031100	1.79739700	0.09660400
C	-4.01003500	-0.28527000	2.73779700
H	-3.05395000	-0.43867100	3.24080600
H	-4.76837300	-0.84825400	3.30777800
H	-3.98456000	-0.73164400	1.74360300
C	-6.76993500	2.24045500	-1.84711800
C	-7.40503500	1.25146400	-2.49736800
H	-7.80887800	0.43784900	-1.89533100
C	-6.20441200	3.47251500	-2.51864600
H	-6.68174700	4.37842500	-2.11928400
H	-5.12809200	3.58695100	-2.34038400
H	-6.35610400	3.47071400	-3.59993200
C	-2.92963000	1.76203900	4.74548000
H	-2.50168700	2.68464500	5.14847100
H	-3.44585100	1.24616300	5.56378300
H	-2.10180500	1.12670100	4.42026000

C	-7.63508500	1.09229800	-3.97316600
H	-7.22156800	1.90767200	-4.57174200
H	-7.18544700	0.15570700	-4.32919900
H	-8.70934200	1.02474100	-4.19321600

TS-EF-6SR-4

l imaginary frequency

H = -5393.917765

G = -5394.123710

E(M06-2X-DCM) = -5394.842319

O	2.26560700	-2.40149500	-0.24377800
O	2.78233900	0.10662500	-0.60650600
P	1.53884200	-0.95690700	-0.51050800
O	0.63923900	-0.52116100	0.60623900
C	5.03307900	-2.90291900	2.85623600
C	5.42928300	-2.39418200	1.62385400
C	4.51171500	-2.27025500	0.56991600
C	2.74559600	-3.13169200	2.01765600
C	3.70484700	-3.28681700	3.03324800
C	3.63814500	0.04867500	-1.70805800
C	4.60572700	-0.95045700	-1.78346500
C	5.27249900	-1.16249200	-3.00003000
C	5.08256200	-0.29550600	-4.07132700
C	4.24753200	0.81191300	-3.90627000
C	3.50682700	1.00905900	-2.73016700
H	3.38556500	-3.70724800	3.98245500
H	4.14818200	1.53983200	-4.70643700
C	5.22625000	-1.83321400	-0.70422900
C	6.47170000	-1.10727400	-0.08189900
H	6.18294200	-0.08343300	0.18265300
H	7.31140900	-1.04634800	-0.78082200
H	7.21493100	-2.12978500	-2.89592300
H	6.00762700	-3.06696700	-3.76785000
C	3.17209300	-2.58651400	0.79152700
H	5.74476900	-3.00390800	3.67176600
H	5.59776900	-0.45464100	-5.01536800
C	6.79390200	-1.89858600	1.20174500
H	7.27673000	-1.28351800	1.96972400
H	7.47383500	-2.73745000	0.99505200
C	6.14874300	-2.39574400	-2.91279000
C	5.70563700	-3.03850900	-1.57659700
H	4.85598700	-3.70877000	-1.74912900
H	6.49779000	-3.61779400	-1.09113000
C	2.71266600	2.26611400	-2.54588100

C	1. 54601300	2. 51656500	-3. 30542900
C	3. 20759000	3. 25556600	-1. 65683900
C	0. 99638700	1. 55639900	-4. 21313700
C	0. 85789200	3. 78132000	-3. 16580600
C	2. 50092500	4. 50854900	-1. 51663600
C	-0. 12939500	1. 83207600	-4. 94410700
H	1. 47014200	0. 58670500	-4. 29320900
C	-0. 31105500	4. 02989600	-3. 95158500
C	1. 34596600	4. 73606100	-2. 27069700
C	-0. 78907500	3. 08788700	-4. 82151300
H	-0. 53465000	1. 07668700	-5. 61011200
H	-0. 80963500	4. 99038500	-3. 84100800
H	0. 81800900	5. 68030100	-2. 15867500
H	-1. 67753400	3. 28911000	-5. 41469800
C	1. 34472900	-3. 58911400	2. 27660200
C	0. 56612300	-2. 93833200	3. 26372700
C	0. 84283800	-4. 73999100	1. 62060400
C	0. 99820600	-1. 74528200	3. 92949900
C	-0. 72357700	-3. 47927900	3. 62889700
C	-0. 46474400	-5. 24751000	1. 96885000
C	0. 24322300	-1. 15873500	4. 91296700
H	1. 93803600	-1. 29308800	3. 63668200
C	-1. 47405900	-2. 84688700	4. 67069400
C	-1. 20566200	-4. 61251000	2. 96908500
C	-1. 00461500	-1. 72565900	5. 30288600
H	0. 59537200	-0. 25055000	5. 39227400
H	-2. 42577800	-3. 28945700	4. 95845900
H	-2. 17665500	-5. 01834300	3. 24769500
H	-1. 57792800	-1. 26516600	6. 10369200
C	4. 86335100	4. 06831200	-0. 04871800
H	5. 78029100	3. 91206300	0. 51357100
C	4. 41009400	3. 09059800	-0. 89570000
H	4. 97613300	2. 17269200	-1. 00311300
C	4. 14879400	5. 28987600	0. 10127900
H	4. 51927100	6. 05291400	0. 78065400
C	3. 00307100	5. 50080900	-0. 61716700
H	2. 44957000	6. 42976400	-0. 51576300
C	1. 08076000	-6. 57555500	0. 02564900
H	1. 67031000	-7. 09918700	-0. 72205100
C	-0. 21664200	-7. 05807700	0. 35784700
H	-0. 60617400	-7. 94198400	-0. 14016300
C	-0. 96276300	-6. 41167700	1. 30493600
H	-1. 95204300	-6. 77372600	1. 57542300
C	1. 59143300	-5. 46072800	0. 63617500

H	2.58310400	-5.11211200	0.37331600
C	-5.56676800	-0.43940600	-0.57110600
C	-5.92493400	-0.20742300	0.92875900
H	-6.32056100	0.80769000	1.02508100
H	-6.74973600	-0.88184600	1.19973300
C	-4.87077900	-0.39104700	1.98348300
C	-4.43005600	0.54697100	-0.97032300
H	-4.82508200	1.55684700	-0.86695500
H	-4.16929300	0.39338700	-2.02187700
N	-3.16399800	0.49372700	-0.21577900
C	-2.60466800	1.55473900	0.42218600
N	-1.27724900	1.50929200	0.64540900
C	-0.50982100	2.46760500	1.37034000
C	-0.57286100	3.83303400	1.07882900
C	0.37385100	1.99971900	2.34591200
C	0.20989700	4.72885200	1.80507000
C	1.16651900	2.90879500	3.04946900
H	0.45522100	0.93431500	2.52672800
C	1.08235000	4.27597300	2.79504000
H	1.70416100	4.97552100	3.33965400
C	2.08062000	2.39838800	4.13144100
C	0.07506500	6.20547900	1.54632400
F	1.39625800	2.14531200	5.27972000
F	3.04672700	3.28644200	4.44366500
F	2.68472600	1.24272800	3.78189500
F	-0.21553800	6.46918400	0.24998800
F	1.20681100	6.87947300	1.85075700
F	-0.91721600	6.75267700	2.28521100
S	-3.59691100	2.83419200	1.04961000
H	-1.21033500	4.19226600	0.28232200
H	-0.72957600	0.66126600	0.40293500
H	-2.48619400	-0.14529500	-0.65311500
C	-4.75197700	0.65975300	2.91811400
H	-5.68539500	1.22227900	3.04441100
H	-4.25867200	1.52746000	2.14783400
N	0.93572200	-1.12045300	-2.00373900
S	-0.52344400	-1.68337300	-2.20921700
O	-1.55945800	-0.60890000	-2.27389300
O	-0.90212900	-2.86782300	-1.42028300
C	-0.41092000	-2.31157900	-3.96115000
F	-0.05532800	-1.35682000	-4.82946500
F	-1.62365600	-2.77251100	-4.31714900
F	0.46625400	-3.31226800	-4.03950800
C	-5.30577800	-1.92669000	-0.88271400

C	-6.20416500	-2.90492400	-0.41211700
C	-4.25313300	-2.35768400	-1.69781500
C	-6.04246300	-4.25237600	-0.72337800
H	-7.05723300	-2.62106000	0.19961500
C	-4.08287000	-3.71159800	-2.00711000
H	-3.53234600	-1.65737000	-2.10074900
C	-4.97311600	-4.66446100	-1.52222500
H	-6.75413800	-4.98002800	-0.34142200
H	-3.23525500	-4.00295800	-2.61736900
H	-4.83799700	-5.71596000	-1.75996500
C	-6.81602500	-0.04496400	-1.46890900
H	-7.55839200	-0.84127500	-1.34813800
H	-6.46819700	-0.12155600	-2.50606300
C	-4.05144000	-1.63243200	2.07395100
H	-3.17824000	-1.51551700	2.71763300
H	-4.68989900	-2.40624900	2.53299800
H	-3.75035700	-2.02585100	1.10299900
C	-7.50456800	1.29831600	-1.25821300
C	-7.09247300	2.38677400	-1.93104800
H	-6.24894700	2.26134300	-2.61159800
C	-8.72509900	1.27590100	-0.36318600
H	-9.50815200	0.64837500	-0.81200600
H	-8.51271100	0.84108700	0.62104900
H	-9.15268700	2.26719500	-0.19864800
C	-3.90701600	0.58444900	4.17908100
H	-3.83506500	1.57774400	4.63170700
H	-4.35660300	-0.08958600	4.91778500
H	-2.88991200	0.23502200	3.98346300
C	-7.64371300	3.78384400	-1.89747200
H	-8.47176600	3.90967700	-1.19558700
H	-6.85796100	4.49889000	-1.62031100
H	-8.00010700	4.08274700	-2.89265700

TS-EF-6SR-5

l imaginary frequency

H = -5393.918232

G = -5394.125016

E(M06-2X-DCM) = -5394.842547

O	2.27056100	-2.41031100	-0.18290200
O	2.80776100	0.08916900	-0.57340000
P	1.55669700	-0.96587400	-0.48284900
O	0.64143200	-0.51005000	0.61297300
C	4.98162500	-2.88024400	2.97163900
C	5.40186400	-2.39347400	1.73835800

C	4. 50291500	-2. 28021800	0. 66734200
C	2. 70676400	-3. 10652700	2. 09848300
C	3. 64790500	-3. 25207000	3. 13230800
C	3. 68199000	0. 00977000	-1. 65913800
C	4. 64433000	-0. 99631900	-1. 70341000
C	5. 33029000	-1. 23032400	-2. 90520500
C	5. 16425000	-0. 37793500	-3. 99206500
C	4. 33381200	0. 73699000	-3. 85738100
C	3. 57439700	0. 95595800	-2. 69713900
H	3. 30979600	-3. 65492400	4. 08261600
H	4. 25290300	1. 45379200	-4. 66956300
C	5. 24125500	-1. 86672800	-0. 60103000
C	6. 48075600	-1. 13908600	0. 03118700
H	6. 19409400	-0. 10966600	0. 27561300
H	7. 33235600	-1. 09370500	-0. 65439300
H	7. 26442900	-2. 20804400	-2. 75430300
H	6. 06579800	-3. 15050400	-3. 63248800
C	3. 15769900	-2. 58445700	0. 87100500
H	5. 67882900	-2. 97315600	3. 80053300
H	5. 69443400	-0. 55406400	-4. 92472600
C	6. 77652100	-1. 91296000	1. 33171000
H	7. 25059000	-1. 28943600	2. 09832300
H	7. 45427100	-2. 75911800	1. 14893800
C	6. 19697900	-2. 46759900	-2. 78513200
C	5. 72747500	-3. 08772300	-1. 44727800
H	4. 87660500	-3. 75528600	-1. 62417100
H	6. 50770000	-3. 66453400	-0. 94002800
C	2. 78562100	2. 22069000	-2. 54519700
C	1. 63567800	2. 46845800	-3. 33071100
C	3. 27057900	3. 21938600	-1. 66097800
C	1. 09630300	1. 49913800	-4. 23481200
C	0. 95458400	3. 74008100	-3. 22287100
C	2. 57076700	4. 47937100	-1. 55272600
C	-0. 01308000	1. 77232700	-4. 99137300
H	1. 56413900	0. 52494700	-4. 29160000
C	-0. 19711900	3. 98568700	-4. 03462100
C	1. 43252600	4. 70430900	-2. 33252600
C	-0. 66547700	3. 03457400	-4. 89986300
H	-0. 41113700	1. 01031600	-5. 65416700
H	-0. 69047500	4. 95127500	-3. 94760300
H	0. 90973200	5. 65391600	-2. 24475800
H	-1. 54085000	3. 23354800	-5. 51291100
C	1. 29824400	-3. 54855500	2. 34218900
C	0. 50949800	-2. 87543400	3. 30607400

C	0.79715100	-4.70572300	1.69680400
C	0.94078100	-1.67514800	3.95928000
C	-0.79042300	-3.39972700	3.65903100
C	-0.52002000	-5.19685700	2.03215900
C	0.17473600	-1.06600000	4.92020200
H	1.88912600	-1.23568600	3.67464500
C	-1.55240800	-2.74392000	4.67774400
C	-1.27141000	-4.53964100	3.00998700
C	-1.08419000	-1.61592600	5.29868700
H	0.52662900	-0.15285700	5.39018100
H	-2.51240400	-3.17383500	4.95705000
H	-2.25010900	-4.93295600	3.27944600
H	-1.66673500	-1.13732300	6.08203100
C	4.90100200	4.04368000	-0.03292500
H	5.80572800	3.88908800	0.54925100
C	4.45689700	3.05698100	-0.87431500
H	5.01812700	2.13362500	-0.95745000
C	4.19282000	5.27240800	0.08548100
H	4.55591000	6.04265200	0.76070900
C	3.06279000	5.48102500	-0.65807100
H	2.51434400	6.41530500	-0.58092100
C	1.04494400	-6.56866600	0.13550200
H	1.64185100	-7.10908600	-0.59419900
C	-0.26158500	-7.03515000	0.45456200
H	-0.65060200	-7.92374100	-0.03544700
C	-1.01721900	-6.36748000	1.37907900
H	-2.01373600	-6.71695200	1.63933200
C	1.55521500	-5.44832200	0.73616400
H	2.55379700	-5.11202900	0.48362100
C	-5.55628200	-0.43440100	-0.64122500
C	-5.95225600	-0.19752300	0.84940100
H	-6.40639700	0.79501300	0.92390200
H	-6.75083700	-0.90760000	1.10763500
C	-4.91374900	-0.33305600	1.92344000
C	-4.41423500	0.54640800	-1.03574400
H	-4.79642300	1.55870500	-0.92912600
H	-4.15265300	0.39427300	-2.08738300
N	-3.15071500	0.49514400	-0.27656600
C	-2.59568800	1.56458000	0.35117200
N	-1.27210200	1.51959600	0.59323500
C	-0.51094800	2.48970000	1.30955100
C	-0.56479100	3.84935300	0.99077300
C	0.35755500	2.03766700	2.30602400
C	0.21080800	4.75643400	1.71086400

C	1. 14398200	2. 95735000	3. 00262800
H	0. 43230100	0. 97573100	2. 50863300
C	1. 06806100	4. 31971800	2. 72104800
H	1. 68485300	5. 02753600	3. 26060900
C	2. 04184800	2. 46477200	4. 10628600
C	0. 08354100	6. 22825700	1. 42240700
F	1. 34151000	2. 23666000	5. 25013200
F	3. 00719400	3. 35525500	4. 41383500
F	2. 64592500	1. 30036600	3. 78719300
F	-0. 17752300	6. 46846400	0. 11529200
F	1. 20870900	6. 90704500	1. 74004200
F	-0. 92480600	6. 78918100	2. 12851800
S	-3. 59014000	2. 86294800	0. 93922100
H	-1. 18962500	4. 19554600	0. 17856700
H	-0. 72350800	0. 66565700	0. 37377100
H	-2. 47040900	-0. 14978200	-0. 70156000
C	-4. 81319000	0. 74503500	2. 82714000
H	-5. 74743000	1. 31253300	2. 91767000
H	-4. 29885900	1. 58665800	2. 03805100
N	0. 97706100	-1. 14702700	-1. 98332200
S	-0. 48134600	-1. 70615100	-2. 20449700
O	-1. 51208400	-0. 62821300	-2. 29492500
O	-0. 87624100	-2. 88115500	-1. 40960000
C	-0. 34512300	-2. 35269300	-3. 94816900
F	0. 03017000	-1. 40940400	-4. 82057900
F	-1. 55490000	-2. 80986000	-4. 31887300
F	0. 52683500	-3. 35953000	-4. 00203800
C	-5. 29035600	-1. 92410100	-0. 94068700
C	-6. 19474300	-2. 90280200	-0. 48281200
C	-4. 22472200	-2. 35649600	-1. 73872300
C	-6. 02804400	-4. 25051400	-0. 79091600
H	-7. 05681500	-2. 62108400	0. 11676400
C	-4. 04875300	-3. 71049800	-2. 04342100
H	-3. 49785200	-1. 65726400	-2. 13253600
C	-4. 94649200	-4. 66326900	-1. 57222400
H	-6. 74557700	-4. 97769500	-0. 41920900
H	-3. 19123900	-4. 00230500	-2. 63933400
H	-4. 80724400	-5. 71495100	-1. 80673400
C	-6. 81175200	-0. 05684600	-1. 53681300
H	-7. 59338800	-0. 78072400	-1. 28666000
H	-6. 52298900	-0. 27482700	-2. 57325600
C	-4. 08455300	-1. 56432000	2. 05811600
H	-3. 20327100	-1. 41498200	2. 68401600
H	-4. 71124300	-2. 31929900	2. 56269000

H	-3.79447500	-1.99809200	1.10114300
C	-7.40514800	1.34267200	-1.46163200
C	-8.49835100	1.55479200	-0.70787500
H	-8.91075200	0.70354300	-0.16281500
C	-6.78186900	2.43406500	-2.31534100
H	-6.11320400	3.08931000	-1.74197300
H	-6.19101000	2.00640000	-3.13191900
H	-7.54463100	3.07576200	-2.76764600
C	-3.98935600	0.71041500	4.10383700
H	-3.91825100	1.71865900	4.52222900
H	-4.45630700	0.06590500	4.85803900
H	-2.97152400	0.34756200	3.93838700
C	-9.25192600	2.84140900	-0.52319800
H	-10.30162300	2.72748800	-0.82649300
H	-9.26596300	3.13669400	0.53500300
H	-8.82365900	3.67194400	-1.08985600

TS-EF-6SR-6

1 imaginary frequency

H = -5393.922704

G = -5394.131588

E(M06-2X-DCM) = -5394.853269

O	-1.21250300	-2.17140900	-1.42522600
O	-2.89222500	-0.60037900	-0.21593000
P	-1.29657500	-0.94428100	-0.33779300
O	-0.61820000	0.29508300	-0.83261000
C	-2.34014000	-1.20857800	-5.34083400
C	-3.29422500	-1.54876900	-4.38676100
C	-2.90178000	-1.95667900	-3.10365800
C	-0.56122500	-1.59171100	-3.69769500
C	-0.98861100	-1.26997600	-4.99856200
C	-3.80549400	-1.59056600	0.14602800
C	-4.25515000	-2.49262400	-0.82071700
C	-5.06347000	-3.57092800	-0.42579000
C	-5.50291400	-3.68970000	0.88764800
C	-5.13628200	-2.71370500	1.81202300
C	-4.27922700	-1.65326900	1.47244300
H	-0.23387500	-1.04060600	-5.74505300
H	-5.50144300	-2.77164900	2.83313700
C	-4.10623700	-2.49813600	-2.34207600
C	-5.25282100	-1.68486500	-3.03227900
H	-5.30500000	-0.69208200	-2.57034900
H	-6.23179000	-2.16070700	-2.91762900
H	-6.35800100	-4.38300100	-1.96386700

H	-5.20955700	-5.55345900	-1.32300000
C	-1.55595500	-1.90345800	-2.74852900
H	-2.63563700	-0.91160800	-6.34421600
H	-6.13132900	-4.52303800	1.19156700
C	-4.80343000	-1.55041800	-4.50462500
H	-5.18854800	-0.64233800	-4.98297800
H	-5.15582200	-2.39698300	-5.11041900
C	-5.33029900	-4.49762300	-1.59099500
C	-4.29687400	-4.02548400	-2.63362200
H	-3.34166900	-4.53539100	-2.46397600
H	-4.59939900	-4.21885700	-3.66745700
C	-3.98042200	-0.63046100	2.52646200
C	-3.24537300	-0.99692500	3.68044900
C	-4.56211400	0.65963700	2.43520900
C	-2.60608300	-2.27058200	3.81650700
C	-3.11109600	-0.05918400	4.77345200
C	-4.39990300	1.59650200	3.52540300
C	-1.91024400	-2.60067900	4.94895700
H	-2.64310700	-2.96374200	2.98661900
C	-2.38977500	-0.45019400	5.94530900
C	-3.68784500	1.20988100	4.66520400
C	-1.80939700	-1.68592600	6.03510300
H	-1.40818600	-3.56145400	5.00898800
H	-2.31005900	0.26297200	6.76283000
H	-3.59495000	1.90826100	5.49542300
H	-1.25698800	-1.96917600	6.92697500
C	0.90337800	-1.61113400	-3.39090700
C	1.67083200	-0.42738000	-3.53430000
C	1.54149400	-2.82766400	-3.03982400
C	1.09585800	0.84140300	-3.87279800
C	3.10190500	-0.47125000	-3.33220600
C	2.96655000	-2.84506700	-2.79816900
C	1.87032300	1.96070100	-4.04352900
H	0.02157700	0.90624100	-3.99540900
C	3.87673100	0.71690300	-3.52824500
C	3.70834100	-1.67135900	-2.95395800
C	3.28431000	1.90057400	-3.87907200
H	1.40261200	2.90407200	-4.31490100
H	4.95398800	0.65121600	-3.39417700
H	4.78207700	-1.68964400	-2.77854500
H	3.88494400	2.79294800	-4.03346800
C	-5.92329300	2.32453100	1.26984500
H	-6.52235200	2.60942300	0.40962300
C	-5.35380900	1.07885400	1.31796300

H	-5.50866100	0.38735100	0.49806500
C	-5.74203500	3.25004200	2.33660300
H	-6.20563100	4.23191100	2.28447600
C	-5.00107600	2.89130200	3.43079300
H	-4.86980400	3.58041300	4.26244200
C	1.48682600	-5.22934200	-2.59061200
H	0.92666500	-6.15769900	-2.51803100
C	2.88462100	-5.23292800	-2.32271600
H	3.37731700	-6.15942400	-2.04086600
C	3.60051300	-4.07210500	-2.42942600
H	4.67097800	-4.05957900	-2.23926300
C	0.84154700	-4.07184500	-2.93827000
H	-0.22169000	-4.09452800	-3.14609900
C	-0.94492700	4.18672700	-0.10595700
C	-1.30871800	3.46619200	1.25274800
H	-2.07916800	4.07078000	1.75496900
H	-1.79592400	2.52241400	0.99812700
C	-0.24954300	3.16061200	2.29164700
C	0.48965200	3.79698000	-0.55808800
H	1.20199500	4.50932200	-0.14912000
H	0.57398100	3.88174600	-1.64567000
N	0.93652700	2.46012800	-0.15805000
C	2.15999400	2.17701200	0.31848000
N	2.55473400	0.89281800	0.32793700
C	3.85088500	0.43816000	0.72985100
C	4.94828200	0.73082900	-0.07657400
C	3.99677200	-0.36231800	1.86415500
C	6.20383900	0.21834500	0.25015700
C	5.26236300	-0.85477700	2.18803500
H	3.13207000	-0.60929900	2.47117500
C	6.36922000	-0.57260700	1.38529400
H	7.34520000	-0.96573700	1.64153800
C	5.41872200	-1.75129500	3.39063300
C	7.34792300	0.49186100	-0.68691800
F	5.10759700	-3.03226700	3.10052900
F	4.61804900	-1.36589400	4.40532700
F	6.69124600	-1.74737200	3.85172700
F	7.13289600	-0.08712100	-1.90014200
F	8.52081000	0.01872500	-0.22355600
F	7.50077000	1.81362100	-0.91962500
S	3.15021400	3.41390800	1.04826800
H	4.81069800	1.33213100	-0.96810600
H	1.91621100	0.14679400	0.02415400
H	0.36377300	1.65619300	-0.47568500

C	0.69049600	4.09217200	2.74422500
H	0.50716100	5.12351200	2.44155800
H	1.73170900	3.82342500	1.93223400
N	-0.89432200	-1.59065000	1.08613500
S	0.58415700	-2.04443000	1.43969800
O	0.96221900	-1.65113900	2.80628300
O	1.57831000	-1.77958500	0.36729600
C	0.46510800	-3.90917600	1.49868400
F	0.04590700	-4.38836300	0.32519500
F	-0.39780200	-4.29324400	2.45269700
F	1.66672100	-4.42254400	1.77874400
C	-2.04340800	3.77036900	-1.11133200
C	-3.36767200	4.19565400	-0.90711200
C	-1.79445800	2.94849500	-2.21859100
C	-4.38761900	3.85210600	-1.79229000
H	-3.62014000	4.80125800	-0.04159300
C	-2.81495500	2.59588500	-3.10535700
H	-0.80597100	2.54582800	-2.40022500
C	-4.11457800	3.05523300	-2.90465900
H	-5.39764800	4.20924100	-1.60937100
H	-2.58767400	1.94829700	-3.94792700
H	-4.90728500	2.78828200	-3.59845200
C	-0.95480900	5.75082300	0.07676600
H	-1.98036000	6.05689700	0.31624300
H	-0.35480000	5.99000100	0.95923100
C	-0.43714100	6.59743800	-1.07770900
C	0.74008400	7.23303700	-0.94006900
H	1.27588100	7.09563500	0.00110200
C	-0.31486100	1.78771100	2.87935300
H	0.59359600	1.48923600	3.40535300
H	-1.13736600	1.76315400	3.61255900
H	-0.56051900	1.02732500	2.13416500
C	-1.31907700	6.71618600	-2.29937500
H	-0.96817000	7.48497000	-2.99144800
H	-1.38315900	5.77120700	-2.85065100
H	-2.34696600	6.96872100	-2.00993400
C	1.39143400	3.98188000	4.09724800
H	2.21521600	4.70066700	4.14589500
H	0.69656100	4.20996000	4.91402300
H	1.81079000	2.98889000	4.27517300
C	1.44781300	8.13010200	-1.91596600
H	2.43502000	7.72025800	-2.16931500
H	0.90028300	8.27462700	-2.85046400
H	1.62720900	9.11975100	-1.47426300

TS-EF-6SR-7

l imaginary frequency

H = -5393.921697

G = -5394.130867

E(M06-2X-DCM) = -5394.854467

O	-0.64590800	-2.63549400	-0.61742200
O	-2.75330400	-1.16119400	-0.26629500
P	-1.11939600	-1.14973600	-0.11008400
O	-0.59755400	-0.04670800	-0.97511200
C	-1.36042800	-3.53759300	-4.64168800
C	-2.34759400	-3.73193400	-3.68085200
C	-2.07442600	-3.50219600	-2.32511900
C	0.19118400	-2.79633900	-2.89607800
C	-0.09730800	-3.10497400	-4.23733200
C	-3.51391100	-2.11732600	0.40958800
C	-3.61263100	-3.41202100	-0.10402800
C	-4.23828000	-4.40580400	0.66712500
C	-4.85381000	-4.09229600	1.87342500
C	-4.85764400	-2.76637900	2.30395800
C	-4.18895900	-1.75626800	1.59396300
H	0.69017900	-2.97791300	-4.97435800
H	-5.37400600	-2.49557100	3.22031100
C	-3.23427900	-3.99068200	-1.46730500
C	-4.41157800	-3.84456100	-2.49101100
H	-4.75401500	-2.80306700	-2.48476300
H	-5.26723200	-4.47885000	-2.23905700
H	-5.07271900	-6.07325500	-0.44025000
H	-3.81933000	-6.54567800	0.70206900
C	-0.84044900	-2.97546800	-1.95436800
H	-1.56149900	-3.72518900	-5.69353500
H	-5.33879100	-4.86243100	2.46788600
C	-3.78280700	-4.17661900	-3.86280500
H	-4.28133500	-3.66139600	-4.69200200
H	-3.84270700	-5.25231900	-4.08032000
C	-4.11599300	-5.75824500	-0.00016100
C	-3.05334200	-5.49886000	-1.08808400
H	-2.05105900	-5.63553700	-0.66633800
H	-3.14489400	-6.16115400	-1.95462100
C	-4.29625400	-0.34625300	2.08819100
C	-3.68196600	0.03799900	3.30434400
C	-5.12647200	0.56833700	1.39219600
C	-2.82783200	-0.83816800	4.04765600
C	-3.90312300	1.36755500	3.82964800

C	-5.31314800	1.90501500	1.91178800
C	-2.25313000	-0.44143700	5.22578000
H	-2.60609500	-1.81707500	3.64361100
C	-3.29563900	1.73654800	5.07161100
C	-4.70024700	2.26602800	3.11535600
C	-2.49670100	0.85844400	5.75344000
H	-1.58426000	-1.11724500	5.74972700
H	-3.48714200	2.73375200	5.46230800
H	-4.86225400	3.26605300	3.51396800
H	-2.03705100	1.15139200	6.69361800
C	1.56352700	-2.32870400	-2.52910500
C	2.06588100	-1.12066600	-3.07564000
C	2.38867300	-3.12946800	-1.70004900
C	1.26661200	-0.23221100	-3.86756200
C	3.43743200	-0.73719900	-2.82363800
C	3.73521700	-2.69733300	-1.40115000
C	1.79644500	0.90813200	-4.41601400
H	0.21882500	-0.46355000	-4.01685500
C	3.95473200	0.45546100	-3.42328200
C	4.22925500	-1.52928800	-1.98774000
C	3.16266100	1.25382000	-4.20491700
H	1.16465500	1.55700000	-5.01741400
H	4.99410100	0.71644300	-3.23726100
H	5.25450600	-1.22698300	-1.78511800
H	3.56881000	2.15367500	-4.65964000
C	-6.64359100	1.12268000	-0.44643400
H	-7.17952200	0.82517700	-1.34383100
C	-5.83938300	0.21893500	0.19913400
H	-5.74659500	-0.78998900	-0.18684700
C	-6.79372900	2.44875400	0.05053600
H	-7.43248400	3.15268500	-0.47593300
C	-6.14773400	2.82251300	1.19829700
H	-6.26908300	3.82568500	1.60095800
C	2.77093800	-5.10800500	-0.31796500
H	2.41345500	-6.04731900	0.09528100
C	4.07696600	-4.64945900	0.01405100
H	4.69791100	-5.23200100	0.68897800
C	4.54515100	-3.48024400	-0.52000100
H	5.53749200	-3.11480100	-0.26890900
C	1.95917300	-4.37662600	-1.14435800
H	0.96875900	-4.74499900	-1.38418600
C	-1.25821300	3.61456400	-1.39817700
C	-1.57935000	3.20413400	0.06728700
H	-2.56905800	3.60867700	0.33581800

H	-1.68255900	2.11915400	0.09071300
C	-0.66546400	3.56560600	1.21606900
C	0.26649300	3.36799000	-1.67923300
H	0.83814700	4.27910200	-1.51369500
H	0.40566900	3.08267700	-2.72525800
N	0.89102400	2.31045000	-0.87300100
C	2.09780800	2.41075000	-0.29907600
N	2.71291700	1.27431800	0.09327500
C	4.07787400	1.14073000	0.45950600
C	5.07846100	1.78750300	-0.26961900
C	4.42544400	0.25619100	1.48750400
C	6.41996500	1.57068100	0.04560400
C	5.77125000	0.03597600	1.77560500
H	3.64760400	-0.26930000	2.02727700
C	6.77829600	0.69657700	1.06890900
H	7.82117300	0.52106800	1.30276000
C	6.15562800	-0.99372700	2.80649100
C	7.46700000	2.28746600	-0.76450500
F	6.38908900	-2.19842700	2.22859100
F	5.19455100	-1.17440200	3.73037800
F	7.29144400	-0.64848900	3.45441400
F	7.22373800	2.16367100	-2.09413200
F	8.70674100	1.80993200	-0.53517800
F	7.48818400	3.61165700	-0.49873300
S	2.77536900	3.97698800	0.07550900
H	4.81872800	2.42333300	-1.10689100
H	2.16920600	0.40209500	0.14189000
H	0.47430700	1.36668500	-0.98060400
C	0.08329100	4.73924600	1.31457700
H	-0.18215200	5.53362000	0.62009300
H	1.24333700	4.36640900	0.70451300
N	-0.85345700	-1.13596800	1.48623000
S	0.59126300	-1.21261600	2.12747100
O	0.72844900	-0.33316700	3.29561000
O	1.70169000	-1.18453100	1.13383800
C	0.67174100	-2.93947400	2.83966000
F	0.48031500	-3.85732400	1.88980600
F	-0.27432200	-3.08984600	3.78088900
F	1.86853200	-3.13412400	3.40280900
C	-2.09573300	2.77594200	-2.40250500
C	-3.09262700	1.86738000	-2.02912600
C	-1.86458900	2.94538500	-3.78093800
C	-3.81837400	1.15406100	-2.98729600
H	-3.32651300	1.68471600	-0.98836400

C	-2.58502000	2.23672600	-4.73995300
H	-1.11038500	3.64812700	-4.12635700
C	-3.57096700	1.33112400	-4.34538100
H	-4.57762400	0.45507800	-2.65123400
H	-2.37544300	2.39618400	-5.79461800
H	-4.13489600	0.77290300	-5.08780900
C	-1.53897000	5.14272300	-1.67772300
H	-0.76821600	5.73883800	-1.18109100
H	-1.38866100	5.31015000	-2.75195500
C	-2.89894500	5.69985800	-1.28267800
C	-2.97375800	6.57142600	-0.26102400
H	-2.04521600	6.83011800	0.25046300
C	-0.61440100	2.57276700	2.33846300
H	0.41623300	2.36132100	2.64820000
H	-1.11545800	2.98375900	3.22650500
H	-1.08785100	1.62193900	2.09506900
C	-4.09429200	5.28768300	-2.11327700
H	-4.93309900	5.97824000	-1.99525700
H	-3.83315300	5.25475000	-3.17720800
H	-4.44969300	4.28438900	-1.85289900
C	0.63539800	5.24206900	2.64442400
H	1.34582400	6.05659400	2.47245100
H	-0.17110400	5.62832100	3.27976200
H	1.15661600	4.45854900	3.20051600
C	-4.18519400	7.26990700	0.29012300
H	-4.05738100	8.36034200	0.25276900
H	-5.10742800	7.02100700	-0.24020000
H	-4.33282900	7.01183300	1.34799200

TS-EF-6SR-8

l imaginary frequency

H = -5393.919775

G = -5394.129273

E(M06-2X-DCM) = -5394.851676

O	-1.06570900	-2.00673000	-1.60750200
O	-2.86164400	-0.76329800	-0.19782400
P	-1.24202100	-0.93598100	-0.37737200
O	-0.69581100	0.41621100	-0.70897900
C	-2.33880100	-0.65497400	-5.35790800
C	-3.24122100	-1.20895300	-4.45576700
C	-2.79243400	-1.74030600	-3.23854400
C	-0.50633100	-1.08220100	-3.78748700
C	-0.98270000	-0.63054200	-5.03122000
C	-3.67400900	-1.87230600	0.03422600

C	-4.05034300	-2.68597900	-1.03659700
C	-4.74673200	-3.87765400	-0.77595200
C	-5.15336200	-4.20041300	0.51368400
C	-4.87134200	-3.31400000	1.55163500
C	-4.12615400	-2.14208500	1.34236300
H	-0.26483600	-0.23186100	-5.74199400
H	-5.21716200	-3.53076100	2.55814300
C	-3.92688200	-2.48729000	-2.54744300
C	-5.15671100	-1.70732900	-3.12378800
H	-5.29626800	-0.79228300	-2.53641900
H	-6.08393300	-2.28650300	-3.06913200
H	-5.98336400	-4.61349500	-2.39739700
H	-4.71757200	-5.73779900	-1.91442100
C	-1.45263800	-1.60589100	-2.88490100
H	-2.67733700	-0.25376100	-6.31004600
H	-5.69392100	-5.12231400	0.71269900
C	-4.74512800	-1.33982900	-4.56741600
H	-5.22151300	-0.41765100	-4.92013700
H	-5.02670600	-2.12983900	-5.27775900
C	-4.94310100	-4.67351700	-2.04726800
C	-3.97760600	-3.97732600	-3.02784500
H	-2.97559700	-4.41036900	-2.92958700
H	-4.27902600	-4.06789800	-4.07602200
C	-3.91764900	-1.21762600	2.50306300
C	-3.10487400	-1.61182300	3.59317600
C	-4.64526800	-0.00227000	2.56307800
C	-2.33555500	-2.81881100	3.58462200
C	-3.02474500	-0.77214500	4.76833300
C	-4.53256400	0.84333500	3.73081800
C	-1.56553500	-3.17941700	4.65809400
H	-2.33744400	-3.43168600	2.69310700
C	-2.22016200	-1.19337900	5.87376200
C	-3.73125200	0.43415800	4.80134600
C	-1.51393600	-2.36432500	5.82421600
H	-0.96756800	-4.08420200	4.60934800
H	-2.18126400	-0.55667600	6.75489900
H	-3.67266700	1.06023000	5.69023400
H	-0.90033900	-2.67073400	6.66708100
C	0.96113600	-1.02246800	-3.50013800
C	1.62873100	0.22829700	-3.48504600
C	1.70220600	-2.22112200	-3.34179100
C	0.94158900	1.48115600	-3.60488500
C	3.06714600	0.27078300	-3.33887100
C	3.13269000	-2.15758700	-3.14353300

C	1. 62596400	2. 66953200	-3. 64451700
H	-0. 14104000	1. 48226000	-3. 65057100
C	3. 74246100	1. 53218000	-3. 38975200
C	3. 77732400	-0. 91811500	-3. 15589400
C	3. 04712300	2. 70102400	-3. 54852400
H	1. 07801500	3. 60218200	-3. 75493700
H	4. 82682700	1. 53503700	-3. 30379900
H	4. 85632200	-0. 87487800	-3. 02117300
H	3. 57183800	3. 65156000	-3. 59723100
C	-6. 24560200	1. 59221200	1. 62163100
H	-6. 92930500	1. 87812300	0. 82654000
C	-5. 54009000	0. 41981800	1. 52684300
H	-5. 66759800	-0. 21559600	0. 65784300
C	-6. 10236800	2. 43816200	2. 75868800
H	-6. 66638800	3. 36530400	2. 81560100
C	-5. 27060600	2. 06823800	3. 78145000
H	-5. 16873000	2. 69298800	4. 66625300
C	1. 84622800	-4. 65859500	-3. 22932700
H	1. 36071500	-5. 62993300	-3. 27077800
C	3. 24951500	-4. 58694200	-3. 00285600
H	3. 82114500	-5. 50080000	-2. 86593100
C	3. 87117100	-3. 36890100	-2. 96733700
H	4. 94422400	-3. 29688300	-2. 80708700
C	1. 10298100	-3. 51981800	-3. 39630300
H	0. 03753300	-3. 59923600	-3. 57659500
C	-1. 14709100	3. 96057300	0. 37243400
C	-1. 39351500	3. 02635000	1. 61138400
H	-2. 26872700	3. 40286800	2. 16433900
H	-1. 68025500	2. 04438300	1. 23148700
C	-0. 32321300	2. 79385400	2. 65745000
C	0. 34365800	3. 83084200	-0. 05326200
H	0. 95852700	4. 53126000	0. 50631300
H	0. 47091000	4. 07821300	-1. 10896300
N	0. 90150500	2. 49085500	0. 15231800
C	2. 14339300	2. 23481800	0. 59017200
N	2. 62089600	0. 98748300	0. 44203200
C	3. 95129300	0. 57430500	0. 76262300
C	5. 01162300	1. 05612200	-0. 00170300
C	4. 17146100	-0. 37272100	1. 76490700
C	6. 30435800	0. 58895000	0. 23486000
C	5. 47287500	-0. 81971700	2. 00064900
H	3. 33634100	-0. 76188600	2. 33812500
C	6. 54345400	-0. 34688900	1. 23896900
H	7. 54799700	-0. 70628300	1. 42477300

C	5. 71367100	-1. 87197200	3. 05377400
C	7. 41008900	1. 08342800	-0. 65688700
F	5. 51545000	-3. 11625500	2. 56855500
F	4. 88818900	-1. 71867500	4. 10903900
F	6. 98365600	-1. 82710200	3. 51961400
F	7. 16835600	0. 75815900	-1. 95581900
F	8. 60894400	0. 56233000	-0. 33157800
F	7. 52342900	2. 42888700	-0. 61703100
S	3. 05212700	3. 43860900	1. 46614100
H	4. 81694600	1. 76867100	-0. 79526300
H	2. 02183200	0. 23671900	0. 07354200
H	0. 37185000	1. 70836500	-0. 27512700
C	0. 52220100	3. 78611700	3. 16886900
H	0. 25265200	4. 80857700	2. 90350200
H	1. 59190300	3. 64814700	2. 38065100
N	-0. 75105900	-1. 71799500	0. 95032800
S	0. 76011900	-2. 12602100	1. 20041900
O	1. 16446400	-1. 88646100	2. 59489900
O	1. 70260100	-1. 67067600	0. 14394500
C	0. 75218900	-3. 98755800	1. 02422200
F	0. 33027500	-4. 34298900	-0. 19120000
F	-0. 06076000	-4. 53900600	1. 93995200
F	1. 98876000	-4. 45682500	1. 21479100
C	-2. 12050800	3. 56893000	-0. 76647700
C	-3. 35567700	2. 96038400	-0. 49739100
C	-1. 85402500	3. 90842700	-2. 10329600
C	-4. 26512100	2. 67462700	-1. 51668400
H	-3. 63439900	2. 68606700	0. 51322000
C	-2. 75781000	3. 62127000	-3. 12641700
H	-0. 93651100	4. 42037500	-2. 37051000
C	-3. 97056300	2. 99651900	-2. 83945400
H	-5. 20417900	2. 19141500	-1. 26276800
H	-2. 51013600	3. 89386500	-4. 14909800
H	-4. 67547400	2. 76942800	-3. 63472800
C	-1. 48114800	5. 45270400	0. 77491900
H	-2. 52654300	5. 44222400	1. 10203400
H	-0. 88397700	5. 71337500	1. 65793100
C	-1. 31030600	6. 55823700	-0. 25449000
C	-2. 39597600	7. 04332700	-0. 87961300
H	-3. 35558200	6. 58793700	-0. 63267400
C	-0. 27082700	1. 39741200	3. 18821600
H	0. 62903600	1. 17922400	3. 76485600
H	-1. 13358400	1. 24851900	3. 85756200
H	-0. 38019300	0. 64766900	2. 40012800

C	0.08912800	7.09360300	-0.46670100
H	0.09258500	8.05376200	-0.98783200
H	0.60187700	7.23926400	0.49324700
H	0.71593300	6.40863500	-1.05260300
C	1.19745400	3.68526600	4.53661600
H	1.94217500	4.48079300	4.63714000
H	0.46436100	3.80602600	5.34264800
H	1.71260000	2.73325900	4.68432200
C	-2.47982900	8.12946800	-1.91322900
H	-3.18851400	8.90884700	-1.60259700
H	-1.52053300	8.61053600	-2.12088800
H	-2.85970200	7.72428000	-2.86131000

TS-EF-6SR-9

l imaginary frequency

H = -5393.920775

G = -5394.129134

E(M06-2X-DCM) = -5394.852025

O	-0.67003600	-2.66695200	-0.46477700
O	-2.72770200	-1.15195200	0.00586000
P	-1.08731500	-1.14689000	-0.00911900
O	-0.65484100	-0.10541900	-0.99134100
C	-1.76025100	-3.75877300	-4.35562400
C	-2.65847500	-3.88579400	-3.30095000
C	-2.25795700	-3.59668300	-1.98912300
C	-0.04074400	-2.97299200	-2.79555800
C	-0.45708000	-3.33912300	-4.08818200
C	-3.42293800	-2.06624800	0.79811300
C	-3.58003400	-3.38236200	0.35888200
C	-4.13755400	-4.33141600	1.23159400
C	-4.63090000	-3.95497600	2.47556000
C	-4.58342700	-2.61055200	2.84081900
C	-3.98018900	-1.64218500	2.02199100
H	0.26304000	-3.26961800	-4.89813300
H	-5.00816100	-2.29105900	3.78803000
C	-3.33920700	-4.02593200	-1.00613300
C	-4.60472800	-3.90484100	-1.92176100
H	-4.92998100	-2.85792000	-1.93248200
H	-5.44185900	-4.51151100	-1.56228700
H	-5.09442200	-6.03248200	0.28744000
H	-3.74114200	-6.47415300	1.32307400
C	-0.98722200	-3.07703300	-1.75818300
H	-2.05972000	-3.99148200	-5.37454200
H	-5.06294000	-4.69055900	3.14931900

C	-4.11114100	-4.31001000	-3.32891500
H	-4.67663900	-3.82244900	-4.13147000
H	-4.20774900	-5.39294700	-3.49018100
C	-4.09573100	-5.71370000	0.61795200
C	-3.14143100	-5.51922200	-0.57838100
H	-2.10458500	-5.65448300	-0.25006000
H	-3.32500100	-6.21680600	-1.40150100
C	-4.03997200	-0.20914800	2.45448300
C	-3.31496800	0.22999000	3.58810300
C	-4.93486700	0.67351600	1.79827500
C	-2.38762000	-0.61051400	4.28285500
C	-3.49359400	1.58083500	4.07431600
C	-5.08238700	2.03041800	2.27656200
C	-1.70453800	-0.16077000	5.38137400
H	-2.20103000	-1.60579900	3.90236300
C	-2.77128100	2.00581000	5.23417600
C	-4.36216500	2.44494900	3.40107800
C	-1.90475100	1.16064700	5.87288400
H	-0.98448000	-0.81125800	5.86822700
H	-2.92786900	3.01991400	5.59535500
H	-4.49412400	3.46026300	3.77107100
H	-1.35758000	1.49620800	6.74979100
C	1.37619300	-2.54194600	-2.58254000
C	1.86912800	-1.38740100	-3.24102400
C	2.25294300	-3.34501200	-1.81004100
C	1.02965600	-0.50287500	-3.99501200
C	3.27543000	-1.06040500	-3.15670900
C	3.64596500	-2.97605800	-1.69532000
C	1.54810100	0.57853900	-4.66123300
H	-0.03733400	-0.68949000	-4.02094200
C	3.77677600	0.07261100	-3.87405300
C	4.12262200	-1.85498100	-2.37989900
C	2.94255600	0.86756100	-4.61383700
H	0.88570000	1.22350200	-5.23318400
H	4.84331300	0.28072500	-3.82031300
H	5.17572500	-1.59119600	-2.30527000
H	3.33704100	1.72034200	-5.15998700
C	-6.61844100	1.14520600	0.08574900
H	-7.23256600	0.80819400	-0.74518100
C	-5.75012600	0.27257900	0.69003700
H	-5.68407600	-0.75048000	0.33751900
C	-6.73525100	2.48914500	0.54205500
H	-7.42794600	3.16726000	0.05084800
C	-5.98839000	2.91330900	1.60787900

H	-6.08133900	3.93135400	1.97960300
C	2.70291800	-5.28780300	-0.39658600
H	2.35104100	-6.18703800	0.10191900
C	4.06697100	-4.90305300	-0.26504600
H	4.74174000	-5.50577200	0.33668100
C	4.52189400	-3.78181000	-0.90307500
H	5.56348200	-3.48030500	-0.82213200
C	1.83183700	-4.54045200	-1.14467700
H	0.80044000	-4.85849400	-1.23899400
C	-1.28974400	3.50631900	-1.73849200
C	-1.50565300	3.25611000	-0.22109600
H	-2.50274700	3.63235200	0.06124500
H	-1.56376000	2.17491100	-0.06406200
C	-0.56570700	3.78019300	0.83444600
C	0.21127800	3.22702300	-2.09693800
H	0.79620500	4.14318100	-2.03422600
H	0.28729700	2.86784600	-3.12623300
N	0.86553600	2.23402600	-1.24225200
C	2.09746200	2.35990900	-0.72377000
N	2.67658600	1.26073000	-0.20937000
C	4.01377100	1.19480700	0.28734000
C	5.07540800	1.31857400	-0.60631300
C	4.25032500	0.91254100	1.63442200
C	6.38491900	1.16072600	-0.15337100
C	5.56684300	0.76985800	2.07650400
H	3.41607300	0.80038000	2.31893900
C	6.63887000	0.89022000	1.18970500
H	7.65615300	0.76929600	1.54121800
C	5.83230700	0.42023000	3.51894200
C	7.50044900	1.26139800	-1.15750200
F	5.81502100	-0.91580800	3.71835600
F	4.90956300	0.95826900	4.34192800
F	7.04620100	0.86263600	3.92167200
F	7.27859700	0.43299300	-2.21342600
F	8.69703600	0.93116900	-0.63330400
F	7.60919100	2.50740300	-1.66723500
S	2.87292800	3.91354100	-0.58771700
H	4.87031900	1.50889500	-1.65356100
H	2.14971500	0.38110400	-0.12232000
H	0.42284300	1.29862300	-1.22415600
C	0.25981400	4.91185100	0.70167000
H	-0.03436900	5.59652300	-0.09315700
H	1.31046600	4.43968600	0.12733900
N	-0.65228800	-1.03427600	1.54624000

S	0.86105100	-1.02781000	2.00413600
O	1.13749400	0.03811700	2.98560900
O	1.84646600	-1.17689200	0.90000800
C	1.03586200	-2.61993000	2.96673900
F	0.77233600	-3.66660000	2.18196800
F	0.18792500	-2.63605400	4.00771100
F	2.28404300	-2.72240000	3.43251700
C	-2.21237600	2.56880500	-2.56340400
C	-3.24818400	1.80895700	-2.00781000
C	-2.05318600	2.51142100	-3.96080800
C	-4.07466400	1.01459100	-2.80720300
H	-3.43416400	1.80530200	-0.94151500
C	-2.87422700	1.72154200	-4.76271000
H	-1.28322400	3.10372200	-4.44862000
C	-3.89389500	0.96242700	-4.18598200
H	-4.86055000	0.43655600	-2.33107400
H	-2.71714500	1.70394900	-5.83817800
H	-4.53622300	0.34226100	-4.80537700
C	-1.61578300	4.98554500	-2.18828100
H	-0.82183900	5.65383000	-1.83654300
H	-1.54573200	5.00709600	-3.28057900
C	-2.96362300	5.55574500	-1.75873400
C	-4.06865300	5.28870400	-2.47419200
H	-3.95141500	4.65702000	-3.35377100
C	-0.56143500	2.97860800	2.09515100
H	-0.33296900	3.57679600	2.97932000
H	-1.51802600	2.46907700	2.24093200
H	0.19056600	2.17439100	2.04676100
C	-2.94025400	6.45759300	-0.54454100
H	-3.92463700	6.85931400	-0.29557800
H	-2.56309800	5.94241700	0.34850400
H	-2.26922500	7.31191900	-0.71350400
C	0.87351300	5.61475800	1.91273700
H	1.56476100	6.39140300	1.57215300
H	0.10329600	6.09549500	2.52708100
H	1.44048000	4.92610800	2.54421000
C	-5.48229600	5.72968900	-2.22156400
H	-6.12645600	4.85672600	-2.04831000
H	-5.58787500	6.39581300	-1.36145900
H	-5.88934800	6.24858400	-3.09978100

TS-EF-6RS

l imaginary frequency

H = -5393.924864

G = -5394.130724

E(M06-2X-DCM) = -5394.848707

O	0.86690200	-3.04620200	-0.03525000
O	2.58093100	-1.14096300	-0.36085300
P	0.97335600	-1.45149800	-0.40487500
O	0.30833900	-0.58916900	0.62456600
C	2.88707000	-4.68213000	3.25323000
C	3.52505100	-4.53282400	2.02679300
C	2.84237600	-4.01243600	0.91620400
C	0.85229900	-3.72038200	2.29856400
C	1.55602000	-4.28748600	3.37374800
C	3.37312500	-1.64179600	-1.39860500
C	3.71349000	-2.99152600	-1.42214300
C	4.25158500	-3.53708300	-2.59767400
C	4.58792100	-2.71524900	-3.66858500
C	4.40659900	-1.33548100	-3.54771500
C	3.78834500	-0.76914800	-2.42195400
H	1.04159300	-4.39772200	4.32411200
H	4.72451900	-0.67509800	-4.34938300
C	3.73806500	-4.04545200	-0.31873500
C	5.15052900	-4.04091200	0.36935200
H	5.41796700	-3.00575900	0.61119900
H	5.93243800	-4.44288000	-0.28178400
H	5.41463800	-5.36231500	-2.39050900
H	3.94949100	-5.56287900	-3.34399200
C	1.52389700	-3.58266700	1.06839900
H	3.41737200	-5.08931900	4.11035700
H	5.00727600	-3.13203800	-4.58087300
C	4.96208000	-4.83929300	1.67326400
H	5.66452200	-4.54194000	2.46011000
H	5.10837100	-5.91637500	1.50810600
C	4.36630600	-5.04340700	-2.47348700
C	3.57939700	-5.34309100	-1.17388500
H	2.51797800	-5.48676500	-1.40505700
H	3.93441700	-6.23656300	-0.64975500
C	3.66870600	0.71810100	-2.29420100
C	2.81981000	1.45828000	-3.15155300
C	4.48656600	1.39145100	-1.35004300
C	1.95107300	0.83510100	-4.10399900
C	2.79709900	2.90227700	-3.06350700
C	4.43885000	2.83335900	-1.26137100
C	1.14768000	1.57909200	-4.92890100
H	1.90380600	-0.24555800	-4.14487200
C	1.95215000	3.64153700	-3.95020600

C	3. 59685700	3. 54871700	-2. 11788800
C	1. 15727800	3. 00207100	-4. 86436000
H	0. 48261500	1. 07158400	-5. 62057100
H	1. 96523500	4. 72758000	-3. 88528200
H	3. 55987900	4. 63273000	-2. 04023100
H	0. 52861200	3. 57636500	-5. 54087800
C	-0. 56783000	-3. 30020500	2. 51638100
C	-0. 84688900	-2. 16051000	3. 30742400
C	-1. 62405600	-4. 09595800	2. 01455500
C	0. 18130700	-1. 31812600	3. 84266700
C	-2. 21899500	-1. 80885900	3. 59422700
C	-2. 99205700	-3. 73562000	2. 30986300
C	-0. 11831700	-0. 22522800	4. 61412100
H	1. 21638300	-1. 54944200	3. 61880700
C	-2. 48940100	-0. 65902300	4. 40207100
C	-3. 25237100	-2. 60236400	3. 08665500
C	-1. 47312600	0. 11004700	4. 90155000
H	0. 68422300	0. 39973900	4. 99635900
H	-3. 52744900	-0. 41265500	4. 61479000
H	-4. 28417600	-2. 34199900	3. 31616900
H	-1. 69316800	0. 97924100	5. 51561600
C	6. 16738400	1. 38765400	0. 42852800
H	6. 84196400	0. 83938100	1. 08060600
C	5. 39247900	0. 70846400	-0. 47510500
H	5. 46703600	-0. 37083500	-0. 53768400
C	6. 10358600	2. 80662300	0. 52039400
H	6. 72450500	3. 32779800	1. 24399900
C	5. 26535600	3. 50535800	-0. 30596900
H	5. 20269500	4. 58836500	-0. 24820300
C	-2. 44058700	-6. 04518300	0. 78756100
H	-2. 24097800	-6. 93850700	0. 20200300
C	-3. 78737900	-5. 68592900	1. 08056000
H	-4. 60125600	-6. 31021100	0. 72116200
C	-4. 05109400	-4. 56363300	1. 82006600
H	-5. 07497900	-4. 28365900	2. 05746400
C	-1. 39883900	-5. 27883100	1. 23959400
H	-0. 37847900	-5. 56805900	1. 01432200
N	0. 54942100	-1. 39861300	-1. 95728000
S	-0. 86477400	-1. 22163600	-2. 61448300
O	-0. 76050800	-1. 07216400	-4. 06717700
O	-1. 76832100	-0. 25748600	-1. 91758400
C	-1. 73020600	-2. 86241900	-2. 36760100
F	-0. 94182500	-3. 86916200	-2. 75178200
F	-2. 85718000	-2. 89777400	-3. 08715000

F	-2.03898600	-3.02550700	-1.07038000
C	-5.04148700	1.42703400	-0.86205600
C	-4.35919500	2.02009800	-2.16001800
H	-5.17055300	2.32192700	-2.83973200
H	-3.83845200	1.19421000	-2.64842000
C	-3.39533300	3.18150000	-2.09977000
C	-4.07904600	1.49527200	0.36184800
H	-4.30793600	2.38504400	0.94357400
H	-4.26422800	0.64680700	1.02680200
N	-2.64320400	1.55000600	0.06810200
C	-1.77824000	2.39314400	0.67794000
N	-0.49287400	2.00808200	0.72110300
C	0.62137200	2.72345200	1.23840100
C	0.88788400	4.06056200	0.92923600
C	1.50760500	2.00530100	2.04646900
C	2.00857100	4.68180400	1.47863400
C	2.62785800	2.63940900	2.58094600
H	1.31366500	0.95778400	2.24514000
C	2.88103500	3.98292200	2.31473800
H	3.74803700	4.47370200	2.73907500
C	3.52360000	1.86070100	3.50776900
C	2.32087900	6.10853800	1.11465100
F	2.99342500	1.79101500	4.75854000
F	3.69742300	0.59127500	3.09149100
F	4.74260500	2.42680400	3.63218000
F	2.89819700	6.77181800	2.13863300
F	3.18599600	6.18792800	0.06774400
F	1.21596400	6.79441600	0.75214800
S	-2.32815100	3.92416500	1.29345800
H	0.22806700	4.61579000	0.27796800
H	-0.28646400	0.99748300	0.56042400
H	-2.23325000	0.74481400	-0.42400400
C	-3.66470900	4.37859000	-1.42317200
H	-4.70394300	4.50843600	-1.11866800
H	-3.14707100	4.11627700	-0.23781300
C	-6.32050000	2.25972900	-0.47147200
H	-7.04327500	2.18158700	-1.29254200
H	-6.03144500	3.31307000	-0.42007200
C	-5.45112700	-0.01110200	-1.25617500
C	-4.84645700	-1.15843900	-0.72618000
C	-6.44593100	-0.19749400	-2.23334800
C	-5.24919800	-2.43758700	-1.12045800
H	-4.03672300	-1.08628700	-0.00870400
C	-6.84823000	-1.47016800	-2.63234500

H	-6.92287800	0.66081900	-2.69832200
C	-6.25745000	-2.60056300	-2.06696500
H	-4.75219600	-3.30146900	-0.69142200
H	-7.62346200	-1.57544800	-3.38688000
H	-6.56794600	-3.59541300	-2.37408900
C	-7.01411100	1.91139500	0.83861200
C	-6.93222600	2.77697900	1.86492300
H	-6.35261500	3.68839000	1.70632900
C	-7.80935200	0.62699100	0.88403200
H	-8.47369400	0.55293700	0.01396400
H	-7.16182500	-0.25627400	0.84699800
H	-8.42622400	0.55350200	1.78245900
C	-7.53720800	2.67401800	3.23650800
H	-6.75272700	2.69358300	4.00519600
H	-8.19022900	3.53393600	3.43842600
H	-8.12443300	1.76488700	3.38640200
C	-2.14142700	2.99992000	-2.89494700
H	-1.36196300	3.72795200	-2.66401700
H	-1.74680900	1.98449600	-2.79585400
H	-2.39537900	3.12870500	-3.96003800
C	-2.97261500	5.69939900	-1.75468800
H	-3.33271700	6.09880700	-2.70993300
H	-3.19383700	6.43678100	-0.97712700
H	-1.88573500	5.60349800	-1.81599100

TS-EF-6RS-1

l imaginary frequency

H = -5393.916670

G = -5394.124067

E(M06-2X-DCM) = -5394.848652

O	2.42711500	-1.66326900	-0.31837800
O	1.80033900	0.50948300	-1.60065700
P	1.25765600	-0.53789100	-0.45037800
O	1.05243300	0.29362200	0.78305900
C	6.38385600	-0.58692100	0.51763200
C	5.89022700	-0.51852400	-0.78081400
C	4.58273900	-0.93559400	-1.07478500
C	4.22503100	-1.44429600	1.28867600
C	5.55963000	-1.07467300	1.53032300
C	1.93005100	0.07067000	-2.92017300
C	3.03331000	-0.69925300	-3.28451500
C	3.05161400	-1.31166900	-4.54841800
C	2.05672200	-1.04403100	-5.48147100
C	1.03927400	-0.15015500	-5.14728300

C	0.94118800	0.41292600	-3.86477400
H	5.94253900	-1.16394400	2.54258500
H	0.28065200	0.10527500	-5.88124000
C	4.36793000	-0.94877900	-2.58530700
C	5.41516600	0.13509600	-3.01934900
H	4.96417400	1.12696700	-2.89569300
H	5.71102100	0.03416500	-4.06778100
H	5.00763000	-1.82422800	-5.34282700
H	3.96361300	-3.21712800	-5.08121300
C	3.74753200	-1.33002500	-0.03090800
H	7.40077600	-0.27564500	0.74330100
H	2.07240900	-1.51192900	-6.46252700
C	6.58720200	-0.02872000	-2.03039600
H	7.13971200	0.90395000	-1.86779100
H	7.31633300	-0.76685600	-2.39324000
C	4.24182300	-2.23901800	-4.67257000
C	4.75019100	-2.32860500	-3.21622800
H	4.20470700	-3.11675500	-2.68633000
H	5.82059200	-2.54413000	-3.13938100
C	-0.15330000	1.39385600	-3.58080800
C	-1.50884200	0.98292900	-3.59755700
C	0.17093600	2.76369100	-3.40630900
C	-1.90090000	-0.38565900	-3.75421700
C	-2.55721600	1.96804600	-3.44140800
C	-0.88607900	3.72963700	-3.20377400
C	-3.22182200	-0.74689800	-3.79448200
H	-1.13521200	-1.14811000	-3.80786400
C	-3.92400300	1.54962000	-3.50421800
C	-2.21831200	3.30710300	-3.23177100
C	-4.25073200	0.23198300	-3.68580600
H	-3.48612300	-1.79590100	-3.88393500
H	-4.69892000	2.30654900	-3.40438600
H	-3.01107300	4.04147400	-3.10246900
H	-5.29097500	-0.07838000	-3.71576300
C	3.40268100	-1.97340000	2.42040000
C	3.13715600	-1.14589200	3.53972000
C	2.98379600	-3.32769600	2.42220300
C	3.49760700	0.24069500	3.58577900
C	2.47039600	-1.70009100	4.69678200
C	2.27781100	-3.85423600	3.56853400
C	3.27497200	1.00228100	4.70479500
H	3.94581700	0.69498100	2.70994800
C	2.26015900	-0.87285700	5.84583300
C	2.05107900	-3.03248300	4.67554400

C	2. 66026400	0. 43776200	5. 85965700
H	3. 56477900	2. 04968200	4. 70588600
H	1. 78252900	-1. 31673200	6. 71681600
H	1. 54279200	-3. 44389700	5. 54556500
H	2. 50893600	1. 04947500	6. 74565600
C	1. 79587600	4. 59022800	-3. 28705200
H	2. 82464200	4. 93625300	-3. 33939700
C	1. 51421200	3. 25953800	-3. 45959700
H	2. 32003300	2. 56148000	-3. 65646000
C	0. 75340800	5. 52974900	-3. 04630900
H	0. 99510200	6. 58016100	-2. 90860000
C	-0. 54848000	5. 10687200	-3. 01107100
H	-1. 35781600	5. 81562300	-2. 85091100
C	2. 82677200	-5. 52932500	1. 37580700
H	3. 03481200	-6. 18519500	0. 53502500
C	2. 10752100	-6. 03358900	2. 49538000
H	1. 77039500	-7. 06639900	2. 49824500
C	1. 84768900	-5. 21764700	3. 56173100
H	1. 30738400	-5. 59054600	4. 42860100
C	3. 25284200	-4. 22832800	1. 34300200
H	3. 80207900	-3. 86871900	0. 48159400
N	-0. 03253600	-1. 28923500	-1. 06643400
S	-0. 47875600	-2. 82413300	-0. 91795600
O	-1. 85328000	-2. 94450500	-1. 42013500
O	-0. 13813600	-3. 43740900	0. 37320300
C	0. 51961900	-3. 77835500	-2. 19331500
F	0. 50518600	-3. 14335900	-3. 37577500
F	-0. 03011700	-4. 98662400	-2. 35034000
F	1. 79607700	-3. 94002100	-1. 81682200
C	0. 07498600	3. 79767400	2. 20079600
C	0. 18747200	2. 70504600	3. 34336800
H	0. 53801300	3. 22480800	4. 24772600
H	0. 98900500	2. 02228100	3. 05723100
C	-0. 98851300	1. 85931200	3. 76083500
C	-0. 95204600	3. 37406600	1. 10604200
H	-1. 91564000	3. 82915600	1. 32554700
H	-0. 64182300	3. 77325200	0. 13528000
N	-1. 18588800	1. 93477900	0. 96844900
C	-2. 40014300	1. 35611300	0. 87159400
N	-2. 45726900	0. 11897500	0. 33910100
C	-3. 59113700	-0. 75536400	0. 39091900
C	-3. 47141200	-1. 97044900	1. 06543300
C	-4. 77723500	-0. 42568400	-0. 26315600
C	-4. 55625300	-2. 84749800	1. 10019000

C	-5.85530300	-1.30953200	-0.21913400
H	-4.84975700	0.50185200	-0.81585900
C	-5.75283100	-2.52109400	0.46426900
H	-6.59173400	-3.20616700	0.49333100
C	-7.11066900	-0.97809900	-0.98066600
C	-4.45411900	-4.12634100	1.89046200
F	-7.02783000	-1.36868200	-2.27816800
F	-8.19472500	-1.59034400	-0.45881400
F	-7.35559700	0.35014800	-0.99174900
F	-4.82515100	-3.93111800	3.18211700
F	-5.26447100	-5.08686500	1.39468000
F	-3.20023500	-4.60993800	1.91070900
S	-3.81474600	2.12559400	1.52383900
H	-2.53291500	-2.24440000	1.53510200
H	-1.62190800	-0.26676100	-0.12687300
H	-0.35763100	1.34272600	0.76359100
C	-2.23130900	2.39780300	4.13122800
H	-2.22539500	3.47522600	4.30420300
H	-2.84725600	2.36374000	2.99069200
C	-0.43825000	5.16361300	2.78811200
H	0.30427100	5.52978400	3.50776900
H	-1.34457900	4.95902600	3.36556400
C	1.52516300	3.93843400	1.68235400
C	2.51026800	4.48908000	2.52350000
C	1.94018100	3.45241400	0.43685400
C	3.84456600	4.57090500	2.12948200
H	2.24293800	4.85966300	3.50914600
C	3.27750700	3.52977000	0.03892500
H	1.24211400	2.98505400	-0.24602200
C	4.23621300	4.09166100	0.87796600
H	4.57701700	5.00902800	2.80275400
H	3.55632500	3.13306900	-0.93205000
H	5.27591600	4.15001500	0.56754500
C	-0.76296900	6.27443500	1.79965900
C	-2.04405600	6.65602500	1.65229600
H	-2.79496400	6.12997700	2.24468900
C	0.39491400	6.91847100	1.07231500
H	1.21526700	7.14053500	1.76546700
H	0.81253500	6.25636500	0.30452000
H	0.10686800	7.85254300	0.58424600
C	-0.72170200	0.39158900	3.82955500
H	-1.62720500	-0.21124900	3.92144200
H	-0.12305800	0.05245800	2.97805800
H	-0.10350300	0.20270200	4.72297600

C	-3.22596700	1.65519200	5.02358500
H	-2.85587000	1.59139500	6.05329300
H	-4.17711800	2.19563700	5.03945800
H	-3.43258700	0.64214300	4.67001100
C	-2.61078400	7.72892900	0.76605400
H	-3.17167100	8.46554300	1.35716600
H	-1.85090900	8.26659000	0.19375200
H	-3.32408700	7.29904900	0.04958300

TS-EF-6RS-2

l imaginary frequency

H = -5393.924562

G = -5394.131032

E(M06-2X-DCM) = -5394.847790

O	1.45726500	-2.76250400	-0.05025700
O	2.87940500	-0.64307300	-0.46779500
P	1.33426400	-1.13758600	-0.26590600
O	0.77695700	-0.43468800	0.92841400
C	3.83429100	-4.15808300	3.10764300
C	4.39524200	-3.86072100	1.87050500
C	3.59020500	-3.44824700	0.79785300
C	1.62416400	-3.56471100	2.23971500
C	2.45617100	-4.03024200	3.27236200
C	3.59957600	-1.06755900	-1.58442200
C	4.16127500	-2.34255900	-1.59886200
C	4.70047700	-2.83754900	-2.79652300
C	4.80321600	-2.02111400	-3.91784100
C	4.37273000	-0.69618400	-3.83286300
C	3.75157000	-0.19249700	-2.67823100
H	2.00118700	-4.27432600	4.22791600
H	4.49527200	-0.03241700	-4.68373300
C	4.42726600	-3.33755500	-0.47247500
C	5.84163200	-3.07563700	0.15392800
H	5.92927800	-2.00785200	0.38556400
H	6.65556500	-3.33621600	-0.52948600
H	6.19393400	-4.40287000	-2.60603900
H	4.74536300	-4.91306200	-3.46528400
C	2.22449000	-3.25444000	1.00357600
H	4.45639000	-4.48330800	3.93771000
H	5.22845900	-2.39838700	-4.84457700
C	5.85128800	-3.89018900	1.46345400
H	6.51100100	-3.46039500	2.22582200
H	6.19561100	-4.92007300	1.29213400
C	5.10119300	-4.28946900	-2.63700100

C	4. 45569500	-4. 67324800	-1. 28539500
H	3. 42505000	-5. 00890500	-1. 44740400
H	4. 98995900	-5. 47160600	-0. 76030600
C	3. 33822600	1. 24443800	-2. 62160400
C	2. 34726100	1. 74287400	-3. 50276500
C	4. 01216100	2. 12781200	-1. 73905900
C	1. 61970800	0. 90377800	-4. 40717900
C	2. 03182000	3. 15461600	-3. 49892300
C	3. 65952600	3. 52936300	-1. 72207600
C	0. 69509700	1. 42232200	-5. 27493000
H	1. 78869300	-0. 16528200	-4. 37678000
C	1. 06109600	3. 65607400	-4. 42273400
C	2. 68084400	4. 00401900	-2. 59960600
C	0. 41958600	2. 81921700	-5. 29649600
H	0. 14926500	0. 75801400	-5. 93843300
H	0. 85572700	4. 72461300	-4. 42147300
H	2. 42534800	5. 06138500	-2. 58512600
H	-0. 30521200	3. 21450400	-6. 00426800
C	0. 15482700	-3. 45274400	2. 50287700
C	-0. 32066000	-2. 50751700	3. 44450000
C	-0. 74225700	-4. 36778500	1. 89947700
C	0. 53218000	-1. 54678500	4. 08045000
C	-1. 72328400	-2. 48994200	3. 79391900
C	-2. 14433800	-4. 32947500	2. 24799400
C	0. 04673300	-0. 66647900	5. 01362200
H	1. 57854400	-1. 50845800	3. 80197500
C	-2. 18980700	-1. 55261900	4. 76908200
C	-2. 59571000	-3. 39523900	3. 18412900
C	-1. 33293900	-0. 67094600	5. 36954500
H	0. 71622300	0. 05424700	5. 47455500
H	-3. 24701200	-1. 56145100	5. 02523200
H	-3. 64934000	-3. 38396900	3. 45759000
H	-1. 69911600	0. 03306800	6. 11203300
C	5. 69555900	2. 58370000	-0. 02329800
H	6. 49182900	2. 23075800	0. 62673200
C	5. 06569400	1. 70512200	-0. 86551200
H	5. 37419800	0. 66645800	-0. 88109300
C	5. 32053100	3. 95636500	0. 00974400
H	5. 82584700	4. 63822900	0. 68854500
C	4. 33275500	4. 41241700	-0. 82046400
H	4. 03954500	5. 45823000	-0. 80985200
C	-1. 20593300	-6. 25798400	0. 41946000
H	-0. 85424000	-7. 00831600	-0. 28340400
C	-2. 58762700	-6. 20992300	0. 75964800

H	-3.27644500	-6.92538800	0.31816400
C	-3.03871900	-5.27295400	1.65063100
H	-4.08852200	-5.23615300	1.93381500
C	-0.31795800	-5.37306500	0.97235900
H	0.73172700	-5.43092900	0.70874300
N	0.64063400	-0.98046500	-1.72516600
S	-0.89681200	-1.15609900	-2.00100000
O	-1.37320300	-0.27025000	-3.07846300
O	-1.74558900	-1.20435300	-0.77536000
C	-1.06479300	-2.86836200	-2.73275700
F	-0.30851700	-2.96499700	-3.83275200
F	-2.34164900	-3.09046100	-3.06711900
F	-0.67734000	-3.79629000	-1.85520000
C	-5.20324900	0.79782200	-0.90140100
C	-4.46554400	1.48871600	-2.11846800
H	-5.22829300	1.68536100	-2.88922900
H	-3.78387100	0.75373000	-2.55218100
C	-3.70030000	2.77869400	-1.96720100
C	-4.40744900	1.01594000	0.41809200
H	-4.75158800	1.92973600	0.89716700
H	-4.63388100	0.20834400	1.12036300
N	-2.95122800	1.12983900	0.27943800
C	-2.19140400	2.03468500	0.93865300
N	-0.88245000	1.75427600	1.07443100
C	0.11954600	2.61355600	1.61390600
C	0.35587100	3.89330600	1.10792100
C	0.93487900	2.10142700	2.62383300
C	1.38255000	4.66850700	1.64550100
C	1.96592900	2.88359900	3.14455000
H	0.77107500	1.09162200	2.97944500
C	2.19296200	4.17290300	2.66800300
H	3.00015000	4.77308000	3.06844900
C	2.80146500	2.31754000	4.26219900
C	1.58595900	6.06765700	1.13066700
F	2.11505000	2.30644300	5.43491100
F	3.16445800	1.03970600	4.02069100
F	3.92680300	3.03146500	4.47203000
F	0.74232000	6.94694300	1.71783800
F	2.84075700	6.51674600	1.35460300
F	1.36061100	6.15002700	-0.20415000
S	-2.87152000	3.52232300	1.52414500
H	-0.24502200	4.27737500	0.29424600
H	-0.52679800	0.79342500	0.90266600
H	-2.46452800	0.29944500	-0.09855500

C	-4.17142000	3.89049300	-1.24309500
H	-5.22949300	3.84874700	-0.98302200
H	-3.66356200	3.66638100	-0.09350900
C	-6.63159300	1.42673800	-0.68361800
H	-7.22689600	1.22359700	-1.58231100
H	-6.52127300	2.51344100	-0.63074700
C	-5.35596500	-0.68623400	-1.30879600
C	-4.75978400	-1.74674600	-0.61503700
C	-6.11038800	-1.00466800	-2.45305800
C	-4.92129100	-3.06983000	-1.03550600
H	-4.13242800	-1.56926500	0.24949000
C	-6.27865500	-2.32185100	-2.87354300
H	-6.57760700	-0.21518200	-3.03587900
C	-5.68605800	-3.36523000	-2.16090900
H	-4.42457000	-3.86294300	-0.48430100
H	-6.86954300	-2.53015700	-3.76168700
H	-5.80826500	-4.39385500	-2.48882400
C	-7.41574800	0.98370200	0.54410800
C	-7.55317100	1.84147200	1.57084200
H	-7.07784600	2.81951200	1.47377300
C	-2.40220700	2.85279600	-2.70213000
H	-2.61414200	3.18483400	-3.73252300
H	-1.71611800	3.59249300	-2.28183500
H	-1.90726100	1.88163500	-2.78401700
C	-8.05011300	-0.38759900	0.50211600
H	-7.30175600	-1.18665200	0.54438300
H	-8.75465900	-0.54358000	1.32214600
H	-8.59488900	-0.53041900	-0.43974500
C	-3.68921300	5.31445100	-1.52321400
H	-4.07259200	5.67374500	-2.48523600
H	-4.05658300	5.98517800	-0.74092100
H	-2.59966900	5.39590500	-1.54034200
C	-8.28354500	1.64812000	2.86962200
H	-7.59355800	1.75278000	3.71794300
H	-9.05483600	2.41928200	3.00038800
H	-8.76702100	0.67205800	2.95555600

TS-EF-6RS-3

1 imaginary frequency

H = -5393.921928

G = -5394.129142

E(M06-2X-DCM) = -5394.846655

0	1.18703900	-2.85051500	-0.14441900
0	2.80129100	-0.87097200	-0.55224500

P	1. 22171100	-1. 21482800	-0. 30669800
O	0. 77933800	-0. 49942500	0. 92759900
C	3. 51911700	-4. 57555300	2. 88174800
C	4. 06475500	-4. 29443800	1. 63401800
C	3. 26869500	-3. 77068200	0. 60410000
C	1. 34998600	-3. 74266300	2. 11240300
C	2. 16647200	-4. 32021500	3. 09997300
C	3. 43486600	-1. 32827200	-1. 70760700
C	3. 86511200	-2. 65140500	-1. 77977000
C	4. 31015800	-3. 15890800	-3. 01036700
C	4. 45473700	-2. 32125200	-4. 11122900
C	4. 16193600	-0. 96370200	-3. 97247200
C	3. 63496800	-0. 43808700	-2. 78130200
H	1. 72168900	-4. 55057800	4. 06369100
H	4. 32053100	-0. 28846600	-4. 80821200
C	4. 06894700	-3. 70285100	-0. 69263700
C	5. 52290500	-3. 60151000	-0. 11223700
H	5. 72465100	-2. 55535800	0. 14540700
H	6. 28302000	-3. 91969800	-0. 83227700
H	5. 64594600	-4. 86884800	-2. 92013700
H	4. 12498400	-5. 20655100	-3. 73840800
C	1. 93644000	-3. 45088200	0. 86522800
H	4. 13360500	-4. 98658200	3. 67877600
H	4. 80773300	-2. 70881600	-5. 06369700
C	5. 49614300	-4. 45353300	1. 17302900
H	6. 22056200	-4. 11435800	1. 92225500
H	5. 73088700	-5. 50635000	0. 96076100
C	4. 56950100	-4. 64753200	-2. 90687800
C	3. 93612100	-5. 00844300	-1. 54332300
H	2. 87214300	-5. 23547100	-1. 67592000
H	4. 40596200	-5. 87179300	-1. 06122900
C	3. 37029700	1. 03014700	-2. 66868600
C	2. 40830800	1. 65330000	-3. 50128500
C	4. 15724800	1. 81301800	-1. 78469900
C	1. 57089500	0. 92055100	-4. 40317100
C	2. 23936000	3. 08894200	-3. 44796600
C	3. 94873800	3. 24153700	-1. 71543300
C	0. 67921100	1. 55689500	-5. 22586300
H	1. 62927000	-0. 16065900	-4. 40676600
C	1. 29865000	3. 71471800	-4. 32582000
C	2. 99790500	3. 83985600	-2. 54671200
C	0. 54900700	2. 97471700	-5. 20093800
H	0. 04838300	0. 97224200	-5. 88902400
H	1. 20459400	4. 79811700	-4. 28884200

H	2.85219900	4.91666500	-2.49436900
H	-0.15131100	3.46340700	-5.87422300
C	-0.09242100	-3.50254300	2.43336100
C	-0.44362700	-2.54988600	3.42087000
C	-1.09162100	-4.31273100	1.84046500
C	0.51694600	-1.69087800	4.04871200
C	-1.82417100	-2.41905500	3.82926600
C	-2.46932700	-4.16346200	2.25082300
C	0.14992500	-0.80217100	5.02692700
H	1.55065300	-1.73685700	3.72748500
C	-2.16556000	-1.47639300	4.85004200
C	-2.79758400	-3.22412700	3.23201200
C	-1.20959400	-0.69512600	5.43980900
H	0.89931400	-0.16017600	5.48109400
H	-3.20840200	-1.39950000	5.15001100
H	-3.83406800	-3.12976700	3.55119100
H	-1.48121300	0.01370600	6.21750600
C	5.92997800	2.04301800	-0.11438600
H	6.70642100	1.59158500	0.49756900
C	5.18956100	1.25944300	-0.96036900
H	5.39189400	0.19641700	-1.01718900
C	5.69553400	3.44424900	-0.02784400
H	6.28680000	4.04981600	0.65387900
C	4.73401100	4.02323900	-0.81083600
H	4.54737400	5.09199400	-0.75923300
C	-1.78208900	-6.10328700	0.32528700
H	-1.52777600	-6.85642100	-0.41554500
C	-3.13842900	-5.94806200	0.72921600
H	-3.90546000	-6.58598600	0.29799100
C	-3.46728500	-5.00620000	1.66718500
H	-4.49675100	-4.88898800	1.99917000
C	-0.79703000	-5.31837500	0.86472500
H	0.23141600	-5.45825200	0.55271100
N	0.49879600	-0.93957500	-1.73393700
S	-1.05698900	-0.95328800	-1.95762400
O	-1.47939400	0.02175600	-2.97996900
O	-1.86489600	-0.97201900	-0.70406800
C	-1.41531400	-2.60756200	-2.75093300
F	-0.70069600	-2.73222900	-3.87600000
F	-2.71572100	-2.68718300	-3.05573900
F	-1.10002900	-3.60510300	-1.92226400
C	-5.08478600	1.34674300	-0.73534800
C	-4.31126400	2.01362300	-1.94351700
H	-5.06457300	2.30025500	-2.69518000

H	-3.69712500	1.24175200	-2.41249800
C	-3.44671300	3.23353400	-1.76573800
C	-4.26060400	1.48781400	0.57469200
H	-4.49246700	2.44080800	1.04373500
H	-4.56690400	0.71326600	1.28424000
N	-2.80307500	1.44098200	0.42121700
C	-1.94115500	2.24718600	1.08282900
N	-0.66491400	1.83172600	1.18011500
C	0.43106000	2.57143500	1.71423600
C	0.78242100	3.83451000	1.23360300
C	1.21506600	1.95324600	2.68896000
C	1.89443700	4.48859800	1.76229700
C	2.33208500	2.61413700	3.20052800
H	0.95946100	0.95545700	3.02374200
C	2.67572800	3.88683400	2.74991300
H	3.54875800	4.39229200	3.14293300
C	3.13454000	1.93751000	4.28031500
C	2.22536700	5.87401000	1.27730200
F	2.48051900	1.96304100	5.47112000
F	3.36136300	0.63678400	3.99767200
F	4.33087600	2.52966000	4.47597800
F	1.49358800	6.81739400	1.91304500
F	3.52557300	6.18652800	1.47332000
F	1.97185000	6.01725600	-0.04724000
S	-2.45297600	3.77839200	1.72484700
H	0.20362000	4.29838200	0.44594300
H	-0.41125400	0.84625100	0.97213500
H	-2.41633800	0.57089700	0.01649000
C	-3.81586900	4.34713200	-0.98550700
H	-4.86663000	4.36467300	-0.69266100
H	-3.28375600	4.04699200	0.12842600
C	-6.47913300	2.04721100	-0.50803100
H	-7.03553000	1.96085300	-1.44639800
H	-6.31019200	3.11962700	-0.35230200
C	-5.34977200	-0.11655600	-1.15946000
C	-4.93170200	-1.22979200	-0.42215900
C	-6.05140200	-0.36010800	-2.35485300
C	-5.20663200	-2.53032800	-0.85361800
H	-4.35433200	-1.11631200	0.48744600
C	-6.33386800	-1.65358900	-2.78686600
H	-6.38724200	0.47138900	-2.96917100
C	-5.91310000	-2.74990700	-2.03251200
H	-4.84139100	-3.36920500	-0.26857700
H	-6.87709400	-1.80243000	-3.71643900

H	-6.12183600	-3.76170400	-2.36906800
C	-7.35517100	1.53016400	0.62948800
C	-8.26610100	0.57513100	0.37927100
H	-8.32154700	0.19408400	-0.64020100
C	-2.16392500	3.23371000	-2.52908100
H	-2.37988900	3.57492100	-3.55560300
H	-1.42502100	3.92971100	-2.12504200
H	-1.73365900	2.23284100	-2.62357600
C	-7.18113200	2.18985500	1.98103300
H	-7.14901500	3.28277400	1.87761500
H	-7.99650200	1.95132400	2.66754700
H	-6.24734400	1.89768100	2.47794400
C	-3.24861300	5.74609500	-1.23271700
H	-3.64316000	6.16755800	-2.16439700
H	-3.53979800	6.40792100	-0.41175700
H	-2.15750400	5.75526700	-1.29040500
C	-9.22740800	-0.07875000	1.33029700
H	-10.26025100	0.02371500	0.97071300
H	-9.02672200	-1.15703200	1.39308100
H	-9.18302400	0.32466900	2.34506300

TS-EF-6RS-4

l imaginary frequency

H = -5393.923518

G = -5394.131375

E(M06-2X-DCM) = -5394.848336

O	1.42725200	-2.74968800	-0.35525100
O	2.73396100	-0.58061600	-0.88075200
P	1.25743900	-1.11822900	-0.42950100
O	0.93711200	-0.51188500	0.89869200
C	4.34964200	-4.30214300	2.21776600
C	4.67296800	-3.91719700	0.92125700
C	3.68258200	-3.45143800	0.04308400
C	2.01514200	-3.69230800	1.80937800
C	3.02418600	-4.20833900	2.63988200
C	3.23949900	-0.92115200	-2.13563200
C	3.79533000	-2.18300900	-2.33751900
C	4.10682900	-2.59019700	-3.64429700
C	3.99680400	-1.70179100	-4.70872400
C	3.58461400	-0.39221900	-4.45800600
C	3.18564700	0.02551700	-3.17779500
H	2.75318700	-4.52003400	3.64445400
H	3.54645500	0.32753100	-5.27045000
C	4.27064700	-3.24419300	-1.34844600

C	5.77472400	-2.99841200	-0.97588200
H	5.89805600	-1.94627900	-0.69421200
H	6.45060600	-3.20067900	-1.81240100
H	5.61852600	-4.13736400	-3.83674700
H	4.03913300	-4.61693900	-4.44713500
C	2.37740100	-3.29556200	0.50708700
H	5.11513400	-4.66874000	2.89707400
H	4.24528700	-2.01152000	-5.72081000
C	6.02954500	-3.89477600	0.25329300
H	6.81585300	-3.50277300	0.90842400
H	6.34247500	-4.90528400	-0.04592400
C	4.53821800	-4.04197800	-3.65854800
C	4.15574900	-4.52375000	-2.24011000
H	3.11478600	-4.86644500	-2.23151800
H	4.78231400	-5.34465600	-1.87673700
C	2.79217200	1.45116000	-2.95053000
C	1.65684600	1.99624300	-3.59890900
C	3.62232000	2.28263900	-2.15485800
C	0.77072200	1.20951700	-4.40335100
C	1.35406500	3.40280900	-3.44865800
C	3.28520200	3.67783100	-1.98498600
C	-0.29510100	1.77484100	-5.05256200
H	0.93697700	0.14169000	-4.47048700
C	0.23230700	3.95405000	-4.14502300
C	2.16247300	4.19913100	-2.63377600
C	-0.56268300	3.16874000	-4.93667200
H	-0.95693700	1.14908900	-5.64406100
H	0.03548700	5.01894200	-4.03932600
H	1.91954600	5.25201000	-2.50682000
H	-1.40329800	3.60237200	-5.47312300
C	0.61602000	-3.61266900	2.33346000
C	0.30697900	-2.71976300	3.38800100
C	-0.37196800	-4.49724400	1.83670900
C	1.26098300	-1.80014100	3.93499600
C	-1.02448000	-2.71443700	3.95095200
C	-1.70449400	-4.46583000	2.39430800
C	0.93815600	-0.96945700	4.97763000
H	2.25336000	-1.75475600	3.50216100
C	-1.32165700	-1.82804900	5.03434200
C	-1.99358000	-3.57760900	3.43344300
C	-0.37068600	-0.98463800	5.54102300
H	1.68181900	-0.28027800	5.36853900
H	-2.32652100	-1.84560700	5.45099200
H	-2.99550200	-3.56730600	3.85864800

H	-0.60832300	-0.32032100	6.36765200
C	5.59824000	2.64340300	-0.75801900
H	6.50019400	2.25657200	-0.29114100
C	4.81841800	1.81420900	-1.52109000
H	5.11412700	0.78084900	-1.65864700
C	5.24215400	4.00863800	-0.57033300
H	5.86817000	4.65086600	0.04340900
C	4.11885200	4.50812000	-1.17162200
H	3.83745600	5.54907000	-1.04146300
C	-1.07823600	-6.31491000	0.36360700
H	-0.84571100	-7.03814100	-0.41352900
C	-2.39538700	-6.26370900	0.90132200
H	-3.15623000	-6.94384200	0.52751700
C	-2.69457400	-5.36463800	1.88846200
H	-3.69477200	-5.31754400	2.31248000
C	-0.10420000	-5.46358600	0.81485100
H	0.89441200	-5.51973600	0.39690700
N	0.29961400	-0.86545400	-1.71309800
S	-1.25339200	-1.10771400	-1.75703200
O	-1.91905000	-0.20573800	-2.71572200
O	-1.90987000	-1.24321100	-0.42706100
C	-1.45542200	-2.79108600	-2.54847000
F	-0.79242100	-2.82365300	-3.71059100
F	-2.75478900	-3.01982400	-2.79400000
F	-0.98930200	-3.75284100	-1.75276600
C	-5.13089100	0.64500200	0.33799400
C	-4.59223500	1.32804800	-0.95390100
H	-5.43813200	1.41831100	-1.65793600
H	-3.87598000	0.65697400	-1.42851000
C	-3.94769500	2.68823300	-0.93659200
C	-4.11633300	0.86738300	1.51639900
H	-4.38658200	1.75617300	2.08517800
H	-4.16610400	0.01769600	2.20304800
N	-2.71689700	1.02477800	1.10964600
C	-1.86597300	1.94327800	1.61791000
N	-0.55210200	1.68974300	1.49764900
C	0.52687900	2.53211100	1.89299600
C	0.66066200	3.84862500	1.44666300
C	1.51939800	1.96214500	2.69182300
C	1.76855100	4.59872600	1.83972800
C	2.62604800	2.72176400	3.07033000
H	1.42684400	0.92671800	2.99703800
C	2.75625400	4.04548600	2.65626300
H	3.62122600	4.62938900	2.94434000

C	3. 65405100	2. 08692800	3. 96921200
C	1. 87225300	6. 03337600	1. 39716200
F	3. 18091100	1. 94450800	5. 23486900
F	3. 99358000	0. 85051400	3. 54733100
F	4. 78460600	2. 81854100	4. 05087600
F	1. 16537600	6. 86012400	2. 20079800
F	3. 14900400	6. 47697900	1. 40149200
F	1. 38943400	6. 20844900	0. 14215200
S	-2. 45831200	3. 41274300	2. 33409000
H	-0. 08213700	4. 28103000	0. 78981700
H	-0. 22696700	0. 73974200	1. 22109300
H	-2. 30684100	0. 20911700	0. 62614800
C	-4. 31793300	3. 74864300	-0. 09094600
H	-5. 27989600	3. 63064000	0. 40543000
H	-3. 55300900	3. 53562100	0. 92352300
C	-6. 51339600	1. 24421200	0. 81318300
H	-6. 35238600	2. 27553400	1. 13912300
H	-6. 80769600	0. 69599000	1. 71681100
C	-5. 34132700	-0. 87217800	0. 09049000
C	-5. 71271900	-1. 69226800	1. 17153600
C	-5. 25377800	-1. 47680200	-1. 17053700
C	-5. 98293200	-3. 04828500	1. 00420500
H	-5. 81080500	-1. 27178700	2. 16898700
C	-5. 52577700	-2. 83675300	-1. 34372500
H	-4. 96043900	-0. 90796900	-2. 04422800
C	-5. 89296200	-3. 63035200	-0. 26061200
H	-6. 26936300	-3. 64744000	1. 86473200
H	-5. 43434700	-3. 27191400	-2. 33424600
H	-6. 10068100	-4. 68784300	-0. 39719200
C	-7. 67335700	1. 22654900	-0. 17455200
C	-7. 95923000	2. 34433200	-0. 86669500
H	-7. 33370600	3. 22051600	-0. 68529700
C	-2. 86104200	2. 90522400	-1. 94385800
H	-3. 26679300	3. 49096200	-2. 78371600
H	-2. 04583400	3. 51194600	-1. 53312100
H	-2. 45156500	1. 97457100	-2. 34000500
C	-8. 48719200	-0. 04458200	-0. 26493600
H	-8. 75004200	-0. 39966700	0. 73962900
H	-9. 41716400	0. 09695800	-0. 82018800
H	-7. 92893500	-0. 85560100	-0. 74371700
C	-3. 99211900	5. 20329700	-0. 42585700
H	-4. 59681300	5. 55464800	-1. 27036800
H	-4. 21471700	5. 83904500	0. 43621000
H	-2. 93934000	5. 34936300	-0. 68056000

C	-9.05245500	2.57820000	-1.87164500
H	-8.63113700	2.88580800	-2.83845500
H	-9.67336500	1.69725400	-2.04957800
H	-9.71110400	3.39518700	-1.54665900

TS-EF-GRS-5

1 imaginary frequency

H = -5393.924561

G = -5394.131030

E(M06-2X-DCM) = -5394.847787

O	1.45722700	-2.76256100	-0.04995100
O	2.87943900	-0.64317900	-0.46748000
P	1.33427200	-1.13765600	-0.26571100
O	0.77685900	-0.43468300	0.92851500
C	3.83395300	-4.15796100	3.10825100
C	4.39501500	-3.86070600	1.87113700
C	3.59007800	-3.44829100	0.79838900
C	1.62391400	-3.56459400	2.24009600
C	2.45582300	-4.03007000	3.27284700
C	3.59970500	-1.06774300	-1.58401900
C	4.16136900	-2.34276000	-1.59834200
C	4.70065800	-2.83783200	-2.79593100
C	4.80351300	-2.02146100	-3.91728500
C	4.37306500	-0.69651200	-3.83241300
C	3.75182300	-0.19274400	-2.67786100
H	2.00075400	-4.27407000	4.22838200
H	4.49570200	-0.03279300	-4.68330600
C	4.42724700	-3.33769700	-0.47187700
C	5.84156900	-3.07577700	0.15462700
H	5.92922800	-2.00797700	0.38619600
H	6.65555100	-3.33642600	-0.52870200
H	6.19406000	-4.40317800	-2.60523600
H	4.74554400	-4.91338600	-3.46456800
C	2.22435100	-3.25443700	1.00398400
H	4.45597500	-4.48314000	3.93839400
H	5.22882300	-2.39879700	-4.84396400
C	5.85109400	-3.89023800	1.46421000
H	6.51075300	-3.46040600	2.22660400
H	6.19540800	-4.92014200	1.29299300
C	5.10132400	-4.28975300	-2.63629300
C	4.45571000	-4.67343700	-1.28471500
H	3.42507100	-5.00908300	-1.44678300
H	4.98991600	-5.47177600	-0.75953600
C	3.33853100	1.24421000	-2.62133800

C	2. 34764700	1. 74264200	-3. 50259200
C	4. 01243900	2. 12760000	-1. 73878700
C	1. 62013200	0. 90353200	-4. 40702300
C	2. 03225600	3. 15439500	-3. 49883400
C	3. 65985700	3. 52916500	-1. 72189600
C	0. 69560100	1. 42207100	-5. 27486300
H	1. 78907900	-0. 16553300	-4. 37656800
C	1. 06161200	3. 65584600	-4. 42273300
C	2. 68125000	4. 00381600	-2. 59951200
C	0. 42013800	2. 81897400	-5. 29650600
H	0. 14979600	0. 75775200	-5. 93837800
H	0. 85627800	4. 72439200	-4. 42153100
H	2. 42578600	5. 06119000	-2. 58509200
H	-0. 30459600	3. 21425600	-6. 00434700
C	0. 15455900	-3. 45256700	2. 50313000
C	-0. 32097500	-2. 50727400	3. 44466300
C	-0. 74250400	-4. 36761500	1. 89971100
C	0. 53183900	-1. 54651800	4. 08061400
C	-1. 72362300	-2. 48965000	3. 79398400
C	-2. 14460700	-4. 32926400	2. 24813700
C	0. 04634100	-0. 66613900	5. 01369100
H	1. 57822500	-1. 50823100	3. 80221700
C	-2. 19019700	-1. 55225600	4. 76905500
C	-2. 59602400	-3. 39497000	3. 18419300
C	-1. 33335500	-0. 67055600	5. 36951700
H	0. 71581200	0. 05460500	5. 47462300
H	-3. 24742000	-1. 56105200	5. 02513200
H	-3. 64967100	-3. 38366800	3. 45758500
H	-1. 69957200	0. 03351500	6. 11193200
C	5. 69573400	2. 58350300	-0. 02293000
H	6. 49194400	2. 23056100	0. 62717300
C	5. 06589100	1. 70490800	-0. 86514500
H	5. 37435400	0. 66623100	-0. 88065400
C	5. 32076200	3. 95618600	0. 01001500
H	5. 82606300	4. 63806300	0. 68881300
C	4. 33306400	4. 41223700	-0. 82028600
H	4. 03990100	5. 45806400	-0. 80974900
C	-1. 20612400	-6. 25786700	0. 41974200
H	-0. 85440100	-7. 00823200	-0. 28307200
C	-2. 58783600	-6. 20977300	0. 75985100
H	-3. 27663900	-6. 92524900	0. 31836000
C	-3. 03896700	-5. 27275800	1. 65076700
H	-4. 08878500	-5. 23593000	1. 93388700
C	-0. 31816800	-5. 37294000	0. 97265900

H	0.73153200	-5.43083300	0.70910600
N	0.64079200	-0.98061100	-1.72504900
S	-0.89662600	-1.15621400	-2.00104200
O	-1.37289500	-0.27033300	-3.07853700
O	-1.74554100	-1.20448600	-0.77550300
C	-1.06455100	-2.86845700	-2.73285500
F	-0.30820300	-2.96506700	-3.83280100
F	-2.34138600	-3.09055100	-3.06730400
F	-0.67715600	-3.79640500	-1.85529200
C	-5.20318700	0.79776000	-0.90184700
C	-4.46538800	1.48850900	-2.11893600
H	-5.22807600	1.68506800	-2.88978000
H	-3.78368700	0.75346700	-2.55251700
C	-3.70014700	2.77850400	-1.96780100
C	-4.40744100	1.01594300	0.41767200
H	-4.75160500	1.92976500	0.89668100
H	-4.63391100	0.20838400	1.11997500
N	-2.95121400	1.12984000	0.27909900
C	-2.19144600	2.03473900	0.93831700
N	-0.88250300	1.75433600	1.07421700
C	0.11944500	2.61366600	1.61369900
C	0.35581400	3.89336100	1.10759400
C	0.93467700	2.10165400	2.62376600
C	1.38242500	4.66863300	1.64519800
C	1.96566500	2.88389600	3.14450600
H	0.77084100	1.09188700	2.97947700
C	2.19273300	4.17315000	2.66784300
H	2.99986800	4.77338200	3.06831300
C	2.80109400	2.31796500	4.26230000
C	1.58586100	6.06773800	1.13025500
F	2.11451700	2.30687000	5.43491700
F	3.16422600	1.04014800	4.02090800
F	3.92634400	3.03199300	4.47225000
F	0.74227000	6.94709400	1.71739100
F	2.84068100	6.51680600	1.35412500
F	1.36047800	6.15002000	-0.20456000
S	-2.87160800	3.52240900	1.52365400
H	-0.24499500	4.27732800	0.29380900
H	-0.52684500	0.79346500	0.90258600
H	-2.46448600	0.29941700	-0.09878600
C	-4.17125500	3.89036600	-1.24376100
H	-5.22934100	3.84863700	-0.98373700
H	-3.66351100	3.66635100	-0.09417000
C	-6.63151400	1.42675500	-0.68418600

H	-7.22678400	1.22356800	-1.58289000
H	-6.52115000	2.51345700	-0.63140200
C	-5.35594300	-0.68632200	-1.30914200
C	-4.75976400	-1.74679500	-0.61532300
C	-6.11036900	-1.00482100	-2.45338400
C	-4.92126800	-3.06990400	-1.03571900
H	-4.13241000	-1.56926700	0.24919400
C	-6.27863600	-2.32202800	-2.87379400
H	-6.57759100	-0.21537000	-3.03625000
C	-5.68603500	-3.36536700	-2.16110500
H	-4.42454900	-3.86298500	-0.48446600
H	-6.86952800	-2.53038300	-3.76192400
H	-5.80824200	-4.39401000	-2.48896400
C	-7.41574200	0.98386100	0.54354400
C	-7.55322700	1.84175400	1.57016700
H	-7.07789600	2.81978200	1.47300900
C	-2.40213300	2.85249600	-2.70285500
H	-2.61432900	3.18341100	-3.73355800
H	-1.71629100	3.59284800	-2.28334000
H	-1.90684300	1.88143500	-2.78395500
C	-8.05009400	-0.38745000	0.50168500
H	-7.30173400	-1.18649300	0.54410000
H	-8.75468800	-0.54333400	1.32169200
H	-8.59480900	-0.53039800	-0.44019200
C	-3.68906000	5.31431300	-1.52398400
H	-4.07229500	5.67349100	-2.48610600
H	-4.05658800	5.98510600	-0.74182100
H	-2.59951700	5.39581700	-1.54092800
C	-8.28368100	1.64855900	2.86892500
H	-7.59374900	1.75334100	3.71727700
H	-9.05499400	2.41972400	2.99954200
H	-8.76714600	0.67249900	2.95495600

TS-EF-6RS-6

l imaginary frequency

H = -5393.921928

G = -5394.129142

E(M06-2X-DCM) = -5394.846655

O	1.18704100	-2.85051300	-0.14442100
O	2.80129300	-0.87097000	-0.55224200
P	1.22171400	-1.21482500	-0.30669700
O	0.77933800	-0.49942500	0.92760100
C	3.51911700	-4.57555700	2.88174400
C	4.06475600	-4.29444000	1.63401600

C	3. 26869700	-3. 77068100	0. 60409800
C	1. 34998600	-3. 74266500	2. 11240000
C	2. 16647100	-4. 32021900	3. 09996900
C	3. 43486900	-1. 32826700	-1. 70760400
C	3. 86511600	-2. 65140100	-1. 77977000
C	4. 31016200	-3. 15890100	-3. 01036700
C	4. 45474200	-2. 32124300	-4. 11122700
C	4. 16194100	-0. 96369400	-3. 97246800
C	3. 63497200	-0. 43808000	-2. 78129700
H	1. 72168800	-4. 55058400	4. 06368700
H	4. 32053600	-0. 28845600	-4. 80820700
C	4. 06894900	-3. 70284800	-0. 69263800
C	5. 52290700	-3. 60150800	-0. 11223700
H	5. 72465300	-2. 55535700	0. 14540900
H	6. 28302200	-3. 91969500	-0. 83227700
H	5. 64595000	-4. 86884100	-2. 92014000
H	4. 12498800	-5. 20654300	-3. 73841200
C	1. 93644100	-3. 45088200	0. 86522500
H	4. 13360400	-4. 98658700	3. 67877300
H	4. 80773900	-2. 70880600	-5. 06369500
C	5. 49614400	-4. 45353400	1. 17302800
H	6. 22056200	-4. 11436000	1. 92225500
H	5. 73088800	-5. 50635100	0. 96075800
C	4. 56950500	-4. 64752500	-2. 90688000
C	3. 93612400	-5. 00843900	-1. 54332600
H	2. 87214500	-5. 23546700	-1. 67592500
H	4. 40596400	-5. 87179000	-1. 06123400
C	3. 37030200	1. 03015300	-2. 66867900
C	2. 40831400	1. 65330800	-3. 50127700
C	4. 15725200	1. 81302200	-1. 78468900
C	1. 57090100	0. 92056100	-4. 40316500
C	2. 23936600	3. 08895000	-3. 44795600
C	3. 94874200	3. 24154100	-1. 71542100
C	0. 67921700	1. 55690700	-5. 22585600
H	1. 62927500	-0. 16064900	-4. 40676200
C	1. 29865700	3. 71472800	-4. 32581000
C	2. 99791000	3. 83986200	-2. 54670000
C	0. 54901400	2. 97472900	-5. 20092900
H	0. 04839000	0. 97225600	-5. 88901900
H	1. 20460100	4. 79812700	-4. 28882900
H	2. 85220500	4. 91667100	-2. 49435500
H	-0. 15130300	3. 46342100	-5. 87421400
C	-0. 09242200	-3. 50254700	2. 43335700
C	-0. 44362900	-2. 54989200	3. 42086700

C	-1.09162000	-4.31273600	1.84046000
C	0.51694300	-1.69088300	4.04871100
C	-1.82417300	-2.41906300	3.82926200
C	-2.46932600	-4.16346900	2.25081800
C	0.14992100	-0.80217800	5.02692600
H	1.55065000	-1.73686100	3.72748300
C	-2.16556300	-1.47640300	4.85004000
C	-2.79758500	-3.22413500	3.23200800
C	-1.20959900	-0.69513500	5.43980800
H	0.89930900	-0.16018300	5.48109400
H	-3.20840600	-1.39951100	5.15000800
H	-3.83406900	-3.12977800	3.55118600
H	-1.48121900	0.01369500	6.21750600
C	5.92998100	2.04301900	-0.11437500
H	6.70642400	1.59158500	0.49758000
C	5.18956500	1.25944600	-0.96036000
H	5.39189700	0.19642000	-1.01718200
C	5.69553700	3.44425000	-0.02783000
H	6.28680300	4.04981600	0.65389400
C	4.73401500	4.02324100	-0.81082200
H	4.54737800	5.09199700	-0.75921700
C	-1.78208500	-6.10329000	0.32527800
H	-1.52777100	-6.85642300	-0.41555500
C	-3.13842600	-5.94806700	0.72920700
H	-3.90545600	-6.58599200	0.29798100
C	-3.46728300	-5.00620700	1.66717800
H	-4.49674900	-4.88899800	1.99916300
C	-0.79702800	-5.31837700	0.86471800
H	0.23141900	-5.45825200	0.55270300
N	0.49879900	-0.93957000	-1.73393600
S	-1.05698600	-0.95328400	-1.95762400
O	-1.47939100	0.02176500	-2.97996500
O	-1.86489400	-0.97201900	-0.70406900
C	-1.41530900	-2.60755400	-2.75094000
F	-0.70069000	-2.73221700	-3.87600700
F	-2.71571500	-2.68717500	-3.05574700
F	-1.10002400	-3.60509900	-1.92227400
C	-5.08478900	1.34673900	-0.73535900
C	-4.31126800	2.01362100	-1.94352800
H	-5.06457800	2.30025600	-2.69518800
H	-3.69712800	1.24175300	-2.41251100
C	-3.44671800	3.23353300	-1.76574700
C	-4.26061100	1.48781400	0.57468300
H	-4.49247400	2.44081000	1.04372100

H	-4.56691500	0.71326900	1.28423200
N	-2.80308200	1.44098100	0.42121200
C	-1.94116300	2.24718400	1.08282700
N	-0.66492200	1.83172300	1.18011500
C	0.43105100	2.57143300	1.71423700
C	0.78241100	3.83450900	1.23360500
C	1.21505600	1.95324400	2.68896200
C	1.89442600	4.48859700	1.76230100
C	2.33207400	2.61413700	3.20053100
H	0.95945200	0.95545500	3.02374400
C	2.67571600	3.88683300	2.74991800
H	3.54874600	4.39229300	3.14293800
C	3.13452900	1.93750900	4.28031900
C	2.22535500	5.87401000	1.27730700
F	2.48050700	1.96303900	5.47112400
F	3.36135400	0.63678400	3.99767600
F	4.33086400	2.52966100	4.47598400
F	1.49357400	6.81739300	1.91305000
F	3.52556000	6.18653000	1.47332700
F	1.97183900	6.01725600	-0.04723600
S	-2.45298500	3.77838800	1.72484800
H	0.20361000	4.29838000	0.44594400
H	-0.41126200	0.84624900	0.97213400
H	-2.41634300	0.57089700	0.01648600
C	-3.81587500	4.34712900	-0.98551100
H	-4.86663600	4.36466600	-0.69266600
H	-3.28376500	4.04699000	0.12841800
C	-6.47913900	2.04720100	-0.50804500
H	-7.03553900	1.96082800	-1.44640900
H	-6.31020500	3.11962000	-0.35233100
C	-5.34976800	-0.11656100	-1.15947000
C	-4.93169900	-1.22979600	-0.42216500
C	-6.05139200	-0.36011800	-2.35486600
C	-5.20662500	-2.53033300	-0.85362200
H	-4.35433300	-1.11631200	0.48744300
C	-6.33385200	-1.65360100	-2.78687800
H	-6.38723200	0.47137800	-2.96918700
C	-5.91308600	-2.74991500	-2.03251900
H	-4.84138400	-3.36920800	-0.26857800
H	-6.87707400	-1.80244400	-3.71645300
H	-6.12181800	-3.76171400	-2.36907400
C	-7.35516700	1.53016100	0.62948500
C	-8.26607100	0.57509700	0.37929300
H	-8.32150500	0.19402000	-0.64016900

C	-2.16393400	3.23371000	-2.52909500
H	-2.37991400	3.57487300	-3.55562900
H	-1.42504200	3.92974300	-2.12508900
H	-1.73364900	2.23284600	-2.62355700
C	-7.18114800	2.18989600	1.98101100
H	-7.14907900	3.28281300	1.87756300
H	-7.99650300	1.95134900	2.66753800
H	-6.24734400	1.89777500	2.47792300
C	-3.24862500	5.74609500	-1.23272100
H	-3.64316900	6.16755400	-2.16440300
H	-3.53981800	6.40792000	-0.41176200
H	-2.15751500	5.75527300	-1.29040100
C	-9.22736200	-0.07878300	1.33033600
H	-9.02664900	-1.15705900	1.39314900
H	-9.18299100	0.32466400	2.34509000
H	-10.26020700	0.02364500	0.97074700

TS-EF-6RS-7

l imaginary frequency

H = -5393.923518

G = -5394.131374

E(M06-2X-DCM) = -5394.848337

O	1.42720900	-2.74971100	-0.35525200
O	2.73394700	-0.58065500	-0.88074700
P	1.25741600	-1.11825100	-0.42950500
O	0.93708700	-0.51190200	0.89868600
C	4.34958400	-4.30221600	2.21775100
C	4.67291000	-3.91727600	0.92124100
C	3.68252900	-3.45149800	0.04307400
C	2.01509400	-3.69233600	1.80937800
C	3.02413300	-4.20838700	2.63987500
C	3.23948200	-0.92119300	-2.13562700
C	3.79528900	-2.18306000	-2.33752300
C	4.10677600	-2.59024600	-3.64430500
C	3.99676600	-1.70183100	-4.70872600
C	3.58460500	-0.39225100	-4.45799800
C	3.18565100	0.02548400	-3.17778300
H	2.75313400	-4.52007500	3.64445000
H	3.54646000	0.32750400	-5.27043800
C	4.27058900	-3.24425900	-1.34845800
C	5.77467300	-2.99850700	-0.97590200
H	5.89802700	-1.94637800	-0.69422900
H	6.45054700	-3.20078400	-1.81242500
H	5.61844200	-4.13744300	-3.83676900

H	4. 03903700	-4. 61698200	-4. 44715400
C	2. 37735200	-3. 29559900	0. 50708400
H	5. 11507300	-4. 66882900	2. 89705500
H	4. 24523900	-2. 01155900	-5. 72081500
C	6. 02948400	-3. 89487900	0. 25326900
H	6. 81580300	-3. 50289300	0. 90839700
H	6. 34239300	-4. 90539300	-0. 04595200
C	4. 53813600	-4. 04203600	-3. 65856600
C	4. 15566300	-4. 52380800	-2. 24012800
H	3. 11469300	-4. 86648300	-2. 23153400
H	4. 78221400	-5. 34472800	-1. 87676300
C	2. 79221100	1. 45113500	-2. 95050300
C	1. 65689600	1. 99625300	-3. 59886900
C	3. 62238500	2. 28258400	-2. 15482700
C	0. 77074800	1. 20955800	-4. 40331500
C	1. 35414900	3. 40282400	-3. 44859900
C	3. 28530300	3. 67778300	-1. 98493700
C	-0. 29506500	1. 77491600	-5. 05251400
H	0. 93697600	0. 14172700	-4. 47046400
C	0. 23240200	3. 95410100	-4. 14495200
C	2. 16258200	4. 19911700	-2. 63371300
C	-0. 56261200	3. 16882000	-4. 93660700
H	-0. 95691900	1. 14918600	-5. 64401700
H	0. 03560700	5. 01899700	-4. 03924100
H	1. 91968000	5. 25200000	-2. 50674100
H	-1. 40321900	3. 60247900	-5. 47304900
C	0. 61597800	-3. 61266900	2. 33347000
C	0. 30696200	-2. 71975200	3. 38801100
C	-0. 37203200	-4. 49722500	1. 83672900
C	1. 26098900	-1. 80014800	3. 93499600
C	-1. 02449300	-2. 71439800	3. 95097100
C	-1. 70455400	-4. 46578200	2. 39433800
C	0. 93818600	-0. 96945400	4. 97762900
H	2. 25336300	-1. 75478400	3. 50215300
C	-1. 32164400	-1. 82800100	5. 03436100
C	-1. 99361400	-3. 57755100	3. 43347200
C	-0. 37065200	-0. 98460700	5. 54103200
H	1. 68186600	-0. 28028900	5. 36853000
H	-2. 32650500	-1. 84553700	5. 45101800
H	-2. 99553300	-3. 56722600	3. 85868200
H	-0. 60827000	-0. 32028300	6. 36766000
C	5. 59832500	2. 64328400	-0. 75800000
H	6. 50027400	2. 25642600	-0. 29113400
C	4. 81847700	1. 81411800	-1. 52107400

H	5.11416000	0.78075300	-1.65864500
C	5.24227500	4.00852600	-0.57029700
H	5.86831300	4.65073200	0.04344500
C	4.11898000	4.50804200	-1.17157100
H	3.83761200	5.54899800	-1.04139900
C	-1.07834700	-6.31488400	0.36364000
H	-0.84584200	-7.03812300	-0.41349400
C	-2.39549300	-6.26365300	0.90136300
H	-3.15635300	-6.94377200	0.52756600
C	-2.69465600	-5.36457100	1.88850100
H	-3.69485000	-5.31745400	2.31252500
C	-0.10429100	-5.46357700	0.81487400
H	0.89431800	-5.51975000	0.39692400
N	0.29960100	-0.86546800	-1.71310900
S	-1.25340700	-1.10771100	-1.75705000
O	-1.91904900	-0.20573600	-2.71575100
O	-1.90989500	-1.24319200	-0.42708200
C	-1.45545200	-2.79108800	-2.54847500
F	-0.79244500	-2.82367200	-3.71059300
F	-2.75482100	-3.01981100	-2.79401100
F	-0.98934900	-3.75284200	-1.75276100
C	-5.13088500	0.64504600	0.33798500
C	-4.59222100	1.32807800	-0.95391300
H	-5.43811500	1.41834100	-1.65795200
H	-3.87596900	0.65699600	-1.42851500
C	-3.94767200	2.68825900	-0.93661400
C	-4.11632300	0.86741600	1.51638800
H	-4.38656500	1.75620500	2.08517200
H	-4.16609700	0.01772500	2.20303200
N	-2.71688600	1.02480200	1.10963400
C	-1.86595700	1.94330100	1.61789000
N	-0.55208700	1.68975400	1.49763300
C	0.52690000	2.53211500	1.89297700
C	0.66069700	3.84862500	1.44663800
C	1.51941300	1.96214300	2.69180700
C	1.76859100	4.59871800	1.83970400
C	2.62606800	2.72175400	3.07031600
H	1.42685000	0.92671800	2.99702500
C	2.75628600	4.04547400	2.65624500
H	3.62126200	4.62937100	2.94432200
C	3.65406000	2.08691700	3.96920900
C	1.87230600	6.03336500	1.39712800
F	3.18093400	1.94456600	5.23487900
F	3.99353900	0.85047300	3.54737400

F	4. 78464300	2. 81849300	4. 05082700
F	1. 16542900	6. 86012400	2. 20075100
F	3. 14906100	6. 47695900	1. 40146600
F	1. 38950000	6. 20843200	0. 14211200
S	-2. 45828600	3. 41277600	2. 33405900
H	-0. 08209700	4. 28103400	0. 78978800
H	-0. 22696100	0. 73974600	1. 22108800
H	-2. 30683600	0. 20913800	0. 62613800
C	-4. 31790400	3. 74868000	-0. 09097900
H	-5. 27987100	3. 63069400	0. 40539400
H	-3. 55298700	3. 53565100	0. 92349100
C	-6. 51338100	1. 24427700	0. 81317200
H	-6. 35235800	2. 27559800	1. 13910600
H	-6. 80768700	0. 69606400	1. 71680400
C	-5. 34134200	-0. 87213200	0. 09048800
C	-5. 71274800	-1. 69221100	1. 17153700
C	-5. 25379600	-1. 47676400	-1. 17053600
C	-5. 98297800	-3. 04822600	1. 00421200
H	-5. 81083100	-1. 27172400	2. 16898500
C	-5. 52581200	-2. 83671300	-1. 34371800
H	-4. 96044600	-0. 90794100	-2. 04422900
C	-5. 89301100	-3. 63030100	-0. 26060100
H	-6. 26942000	-3. 64737300	1. 86474200
H	-5. 43438300	-3. 27188100	-2. 33423500
H	-6. 10074300	-4. 68779000	-0. 39717600
C	-7. 67334500	1. 22662200	-0. 17456000
C	-7. 95920600	2. 34440400	-0. 86670900
H	-7. 33367200	3. 22058300	-0. 68531700
C	-2. 86100300	2. 90523600	-1. 94386800
H	-3. 26669300	3. 49108700	-2. 78367500
H	-2. 04574200	3. 51184800	-1. 53307100
H	-2. 45160000	1. 97458000	-2. 34008200
C	-8. 48719500	-0. 04450000	-0. 26493600
H	-8. 75004800	-0. 39957500	0. 73963200
H	-9. 41716600	0. 09704800	-0. 82018800
H	-7. 92894900	-0. 85552900	-0. 74371300
C	-3. 99206300	5. 20332500	-0. 42589800
H	-4. 59676300	5. 55468800	-1. 27040000
H	-4. 21463100	5. 83908100	0. 43617100
H	-2. 93928400	5. 34936400	-0. 68061900
C	-9. 05243200	2. 57827900	-1. 87165800
H	-8. 63111300	2. 88588900	-2. 83846700
H	-9. 67334500	1. 69733600	-2. 04959400
H	-9. 71107700	3. 39526800	-1. 54666900

TS-EF-6RS-8

l imaginary frequency

H = -5393.921136

G = -5394.127565

E(M06-2X-DCM) = -5394.848462

O	1.24941300	-2.82741600	-0.32272200
O	2.67960400	-0.74761800	-0.88604500
P	1.17516600	-1.19051200	-0.42371400
O	0.89521800	-0.54452800	0.89481700
C	4.08481100	-4.51398600	2.26315400
C	4.42495300	-4.16839800	0.95988000
C	3.46061700	-3.65656400	0.07827800
C	1.78990800	-3.76925700	1.85441000
C	2.76954500	-4.33332100	2.68884600
C	3.16107000	-1.13539200	-2.13653400
C	3.64028000	-2.43091700	-2.32116400
C	3.92348400	-2.87446000	-3.62253900
C	3.86450700	-1.99613700	-4.69931600
C	3.53177600	-0.66090300	-4.46672900
C	3.16092600	-0.20206300	-3.19210100
H	2.48490600	-4.61257100	3.69917000
H	3.53479700	0.04822300	-5.28933700
C	4.05456900	-3.50456400	-1.31798100
C	5.57204400	-3.34376800	-0.95326300
H	5.75866300	-2.29716100	-0.68618300
H	6.23157000	-3.59702400	-1.78895200
H	5.33870700	-4.51245200	-3.79645700
H	3.73134600	-4.90449200	-4.39609400
C	2.16935900	-3.41528900	0.54465500
H	4.82982900	-4.91620500	2.94506100
H	4.09183600	-2.33441200	-5.70722700
C	5.77757600	-4.23720200	0.28709500
H	6.58892900	-3.88475000	0.93409800
H	6.02750300	-5.26870900	0.00050000
C	4.26672200	-4.34962400	-3.61696900
C	3.86045400	-4.78744300	-2.19091700
H	2.80089000	-5.06703700	-2.17499000
H	4.43785200	-5.63919600	-1.81725800
C	2.85183500	1.24739900	-2.98557400
C	1.75123600	1.84893100	-3.64413100
C	3.72867000	2.04046900	-2.20079500
C	0.82088100	1.10401800	-4.43841000
C	1.53214900	3.27316400	-3.51606100

C	3.47402500	3.45548600	-2.05218600
C	-0.20798900	1.72163500	-5.09953500
H	0.92318800	0.02727500	-4.48851200
C	0.44678100	3.87940900	-4.22439200
C	2.38496500	4.03244300	-2.71114800
C	-0.39189700	3.13070500	-5.00642500
H	-0.90473600	1.12723800	-5.68324300
H	0.31395000	4.95575000	-4.13612100
H	2.20508800	5.09990300	-2.60103000
H	-1.20363400	3.60534900	-5.55256300
C	0.40123700	-3.59419500	2.38301300
C	0.15448500	-2.66727900	3.42457400
C	-0.64328700	-4.42146300	1.90358400
C	1.16766800	-1.80246900	3.95425300
C	-1.17152100	-2.56797700	3.99161000
C	-1.96891200	-4.29557400	2.46430700
C	0.90310000	-0.93701400	4.98493700
H	2.15926700	-1.82746400	3.51794900
C	-1.40679900	-1.64788100	5.06202200
C	-2.19617000	-3.37475700	3.49035300
C	-0.40165700	-0.85955400	5.55259300
H	1.69112900	-0.29117600	5.36271600
H	-2.40901800	-1.59446900	5.48196800
H	-3.19365400	-3.29355500	3.91836700
H	-0.59286200	-0.16868700	6.36943600
C	5.72112000	2.30555300	-0.80598600
H	6.59843900	1.87348200	-0.33191300
C	4.89472800	1.51223200	-1.55813900
H	5.12953100	0.46142500	-1.67996800
C	5.44545400	3.69191900	-0.63890100
H	6.10696400	4.30540300	-0.03307600
C	4.35404200	4.24742300	-1.24962200
H	4.13388800	5.30481900	-1.13518200
C	-1.47046700	-6.21270800	0.46150800
H	-1.28784400	-6.96159700	-0.30457700
C	-2.77976500	-6.06779700	1.00131600
H	-3.58438600	-6.70267400	0.63981800
C	-3.01680400	-5.13608700	1.97497800
H	-4.01046200	-5.01769100	2.40047200
C	-0.44192900	-5.41910600	0.89672000
H	0.54955600	-5.54613600	0.47731700
N	0.23069000	-0.90464000	-1.71030800
S	-1.33555800	-1.04076200	-1.74451200
O	-1.94078000	-0.11760200	-2.72299100

O	-1.99448900	-1.09784600	-0.41010700
C	-1.65936200	-2.72454300	-2.49283000
F	-1.01366500	-2.82927200	-3.66048800
F	-2.97369400	-2.87047400	-2.71870800
F	-1.24900000	-3.69588400	-1.67822200
C	-5.05855000	1.00026800	0.34005700
C	-4.45391500	1.59946500	-0.96284900
H	-5.26540500	1.69135400	-1.70462100
H	-3.76153900	0.87161100	-1.38867800
C	-3.74137900	2.92295500	-0.97839300
C	-4.02615000	1.16271900	1.51481700
H	-4.24003700	2.06668100	2.08381400
H	-4.12054300	0.31803100	2.20242800
N	-2.62175900	1.23789700	1.10139000
C	-1.71640900	2.10953800	1.60144900
N	-0.42116200	1.77119200	1.48013600
C	0.71219800	2.54307800	1.86476200
C	0.92734600	3.84799400	1.41576000
C	1.67351400	1.91008800	2.65454800
C	2.08686900	4.52333100	1.79522900
C	2.83114900	2.59580500	3.02114400
H	1.51647500	0.88319100	2.96212600
C	3.04428000	3.90739900	2.60288900
H	3.94903200	4.43319100	2.88061200
C	3.82332900	1.89723500	3.91290900
C	2.28328700	5.94600600	1.34548900
F	3.36088000	1.80491000	5.18714600
F	4.06467200	0.63432900	3.50192800
F	5.00575100	2.54455700	3.96885700
F	1.65265100	6.82333900	2.15867700
F	3.58842700	6.29750000	1.32398900
F	1.79086800	6.15134500	0.09877800
S	-2.21727500	3.61748900	2.30122600
H	0.20740200	4.32824500	0.76681600
H	-0.16140600	0.79887200	1.21297900
H	-2.26100400	0.39252700	0.63034900
C	-4.05471700	4.01812100	-0.14763000
H	-5.02918400	3.96162600	0.33532300
H	-3.32051900	3.78323600	0.85757200
C	-6.39996900	1.69755300	0.80211600
H	-6.17055800	2.69196400	1.20089300
H	-6.77106600	1.12494500	1.65823300
C	-5.39028200	-0.49912400	0.11405600
C	-5.79356400	-1.28330900	1.21026400

C	-5.38623300	-1.11494500	-1.14373500
C	-6.16628600	-2.61719800	1.06071600
H	-5.83607900	-0.85111900	2.20678400
C	-5.75735400	-2.45323000	-1.29939400
H	-5.07738400	-0.57371200	-2.02951500
C	-6.14996400	-3.21254800	-0.20137000
H	-6.47232100	-3.18870300	1.93324600
H	-5.72570200	-2.89861700	-2.28925500
H	-6.43542700	-4.25355700	-0.32381200
C	-7.51257200	1.82679300	-0.23325800
C	-8.36187000	0.80683900	-0.44105200
H	-8.21000800	-0.09495000	0.15078900
C	-2.64283700	3.06289400	-1.98451500
H	-2.98499200	3.71591700	-2.80212400
H	-1.77249700	3.57288900	-1.55328500
H	-2.32302100	2.10918900	-2.40690600
C	-7.62153200	3.16819900	-0.92468700
H	-6.70953700	3.42965000	-1.47727100
H	-8.45192300	3.21334500	-1.63226300
H	-7.77521700	3.96901900	-0.18722800
C	-3.65101900	5.44529600	-0.51687600
H	-4.23404400	5.80808400	-1.37163200
H	-3.84127100	6.11205800	0.32919500
H	-2.59095700	5.52739000	-0.77013700
C	-9.51537300	0.72126300	-1.39959400
H	-9.37842700	-0.12574400	-2.08515800
H	-10.45352100	0.53366600	-0.85964600
H	-9.65331500	1.62068800	-2.00502000

TS-EF-6RR

l imaginary frequency

H = -5393.928158

G = -5394.134238

E(M06-2X-DCM) = -5394.852596

O	2.13010800	-2.42466200	-0.42177600
O	2.86600600	0.02659400	-0.79236300
P	1.54745000	-0.89134900	-0.48904700
O	0.95627800	-0.43403400	0.80389500
C	5.02607600	-3.26313300	2.49369000
C	5.38924200	-2.72880800	1.26258700
C	4.42826700	-2.51082900	0.26325700
C	2.68700800	-3.30887200	1.77487000
C	3.68720300	-3.57297100	2.72615200
C	3.58304400	-0.13595500	-1.97754600

C	4.49446800	-1.18487100	-2.08994800
C	5.07631700	-1.45607300	-3.33819100
C	4.85903900	-0.61005700	-4.42008700
C	4.05686800	0.51725300	-4.24572500
C	3.38891100	0.77453400	-3.03605300
H	3.39067300	-4.01143900	3.67447300
H	3.91807300	1.21279700	-5.06796500
C	5.11358900	-2.09603000	-1.03395800
C	6.42299400	-1.45240800	-0.45919300
H	6.20449900	-0.42052100	-0.16087700
H	7.23189700	-1.42215100	-1.19559700
H	6.97763400	-2.50331600	-3.30519100
H	5.69734600	-3.39499000	-4.11932400
C	3.08317000	-2.74446800	0.54634600
H	5.77045900	-3.43955800	3.26604700
H	5.31802000	-0.80988000	-5.38515700
C	6.75819500	-2.29256000	0.79033200
H	7.30341900	-1.72218300	1.55097600
H	7.38610400	-3.15790500	0.53476200
C	5.90135600	-2.72399400	-3.27690000
C	5.48536200	-3.33174700	-1.91858300
H	4.59213700	-3.95365000	-2.04742300
H	6.26332300	-3.95309800	-1.46372500
C	2.56250500	2.01531700	-2.91229400
C	1.45788800	2.22167100	-3.77705500
C	2.95382400	3.03568800	-2.00701100
C	0.98463600	1.22091000	-4.68619600
C	0.75781600	3.48701400	-3.75492400
C	2.20614500	4.27206500	-1.95580200
C	-0.05188600	1.46945700	-5.54712500
H	1.44257400	0.23994300	-4.66537600
C	-0.31176000	3.71074200	-4.67888500
C	1.13955400	4.46859300	-2.83702000
C	-0.69990700	2.73695800	-5.55983200
H	-0.39633400	0.68519900	-6.21499200
H	-0.80331300	4.68159300	-4.66944200
H	0.60442200	5.41646900	-2.81749000
H	-1.50837400	2.92185500	-6.26282200
C	1.27219600	-3.66655100	2.10302900
C	0.60342500	-2.99697500	3.15671700
C	0.64423000	-4.74525200	1.43283600
C	1.18104100	-1.89665400	3.87126700
C	-0.72067100	-3.42505100	3.54776100
C	-0.68877600	-5.14739700	1.81948000

C	0.52047600	-1.29258300	4.91053900
H	2.15650000	-1.53058500	3.57358600
C	-1.37757000	-2.76415900	4.63362200
C	-1.33122200	-4.48125800	2.86678300
C	-0.77618800	-1.73340500	5.30303600
H	0.98556300	-0.46094300	5.43239100
H	-2.37031500	-3.10655500	4.91751800
H	-2.32692600	-4.80158500	3.16737300
H	-1.28384700	-1.24327200	6.12954200
C	4.43369400	3.92133800	-0.27208900
H	5.30207600	3.80188900	0.37037600
C	4.09162900	2.92156900	-1.14453500
H	4.69662400	2.02408800	-1.19058600
C	3.66429200	5.11638000	-0.19480100
H	3.93364900	5.88992400	0.51813700
C	2.58645800	5.28520400	-1.02084700
H	1.99156800	6.19343000	-0.97572500
C	0.65602900	-6.54042300	-0.22636100
H	1.16901000	-7.09062000	-1.01067300
C	-0.66675000	-6.91602800	0.14214100
H	-1.15301500	-7.74465500	-0.36570600
C	-1.31462600	-6.23886400	1.13944300
H	-2.32028300	-6.52303300	1.44068500
C	1.28731600	-5.49644500	0.39734000
H	2.29717000	-5.22998700	0.10757600
N	0.68285500	-0.85540900	-1.86267600
S	-0.81557100	-1.29340900	-2.01313300
O	-1.53304700	-0.47780500	-3.00967900
O	-1.54220200	-1.53382900	-0.73090900
C	-0.76456100	-2.99703800	-2.77700900
F	-0.21517700	-2.94280800	-3.99462600
F	-2.01871900	-3.46349400	-2.88978600
F	-0.05888900	-3.83195200	-2.01440600
C	-5.08344800	-0.10390200	-0.56332600
C	-4.40321300	0.72735800	-1.69130500
H	-5.02571300	0.68659500	-2.60082400
H	-3.47995800	0.22558300	-1.99294900
C	-4.09286000	2.17860000	-1.50889900
C	-4.32373400	0.13734900	0.78457900
H	-4.79404900	0.93978100	1.34739600
H	-4.39155700	-0.76514700	1.39970300
N	-2.91144100	0.50508400	0.65388900
C	-2.31009500	1.50440300	1.33815400
N	-0.96442500	1.45844600	1.40517900

C	-0.09337500	2.39467700	2.03128100
C	-0.13846900	3.76828700	1.77592000
C	0.89315600	1.87572500	2.87193600
C	0.77987200	4.61350100	2.39681100
C	1.81045500	2.73306500	3.47953800
H	0.94533300	0.80574100	3.03179200
C	1.75719200	4.10651500	3.25535300
H	2.47568800	4.76884200	3.72254300
C	2.82951700	2.14604700	4.41966400
C	0.69428100	6.09892300	2.16966200
F	2.26926000	1.81479200	5.61232700
F	3.37637100	1.01413300	3.92580800
F	3.83572200	3.00528300	4.68388100
F	1.91279800	6.68625200	2.20660600
F	0.13751300	6.39943800	0.97260600
F	-0.05893300	6.70768600	3.11371800
S	-3.22764300	2.79939200	2.03784600
H	-0.87233300	4.17437300	1.09402000
H	-0.46343300	0.60114400	1.10169300
H	-2.30286100	-0.20472000	0.21708500
C	-4.80926200	3.02677900	-0.63714400
H	-5.77931400	2.63040100	-0.32891500
H	-4.16779400	2.86062800	0.42068300
C	-4.95656700	-1.60672600	-1.04775000
H	-3.91697400	-1.77362500	-1.34355800
H	-5.55832400	-1.68745100	-1.96074900
C	-6.58275000	0.22199700	-0.38896700
C	-7.20400000	0.23661200	0.87085300
C	-7.40736900	0.43013800	-1.50891700
C	-8.57308900	0.47834300	1.00754800
H	-6.62993400	0.04342400	1.76982100
C	-8.77474700	0.67079400	-1.37838900
H	-6.98993000	0.39469200	-2.51119500
C	-9.36686900	0.70228600	-0.11520800
H	-9.01553600	0.48424900	2.00010200
H	-9.37658500	0.83205000	-2.26890900
H	-10.43141800	0.89180800	-0.01009200
C	-5.35867400	-2.70792700	-0.07385200
C	-6.65077400	-3.04587300	0.07481100
H	-7.38338500	-2.49365100	-0.51357500
C	-2.94660200	2.71213000	-2.30538600
H	-2.25609800	3.27129000	-1.65886300
H	-2.38672400	1.92968400	-2.81988600
H	-3.31143000	3.44053300	-3.04362600

C	-4.20652600	-3.42596800	0.59267500
H	-3.57211700	-3.90635000	-0.16378900
H	-3.54005200	-2.74298200	1.13285700
H	-4.53469700	-4.19567500	1.29517600
C	-4.78606400	4.54497200	-0.80834400
H	-5.35239400	4.84614500	-1.69744000
H	-5.24639100	5.02122800	0.06199400
H	-3.76957200	4.93688500	-0.90159500
C	-7.24763500	-4.11184600	0.95029300
H	-8.00250200	-3.68103000	1.62225100
H	-7.76800700	-4.86678000	0.34448200
H	-6.51035800	-4.63191100	1.56695900

TS-EF-6RR-1

l imaginary frequency

H = -5393.928142

G = -5394.135446

E(M06-2X-DCM) = -5394.852340

O	2.02142700	-2.50973200	-0.38062400
O	2.88957900	-0.10346300	-0.76038100
P	1.52197000	-0.94823600	-0.46374000
O	0.94529500	-0.45385400	0.82270300
C	4.84486100	-3.47096100	2.56791600
C	5.24596100	-2.97055900	1.33432100
C	4.30586400	-2.71146900	0.32503200
C	2.51208700	-3.39622400	1.83107000
C	3.48927500	-3.70387500	2.79316700
C	3.60475000	-0.31333300	-1.93968400
C	4.46013000	-1.40976200	-2.03726400
C	5.03502800	-1.72161400	-3.27923400
C	4.86913400	-0.87463200	-4.36944300
C	4.12521200	0.29417500	-4.21013300
C	3.46391800	0.59624300	-3.00726700
H	3.16208700	-4.11397400	3.74409500
H	4.02717300	0.98838600	-5.03935000
C	5.02216000	-2.34448000	-0.96994300
C	6.35967500	-1.76697200	-0.38973400
H	6.19420500	-0.72249200	-0.10129800
H	7.17463100	-1.78599400	-1.11980800
H	6.87808200	-2.86749200	-3.22346400
H	5.55855500	-3.69674600	-4.04099800
C	2.94803000	-2.86970400	0.59928300
H	5.57265900	-3.67927400	3.34810000
H	5.32308100	-1.10649300	-5.32971900

C	6. 63996600	-2. 61330500	0. 86909300
H	7. 20997200	-2. 06691800	1. 62916900
H	7. 22163800	-3. 51365500	0. 62520200
C	5. 79146900	-3. 03083100	-3. 20205600
C	5. 33376100	-3. 60502200	-1. 84255100
H	4. 40949900	-4. 17924900	-1. 97375300
H	6. 07404600	-4. 26350400	-1. 37714700
C	2. 69907100	1. 87728700	-2. 89924900
C	1. 60760000	2. 12815600	-3. 76881200
C	3. 13698100	2. 88589800	-2. 00230600
C	1. 09080700	1. 14387400	-4. 67223400
C	0. 96665600	3. 42457400	-3. 75735800
C	2. 44898800	4. 15685700	-1. 96374300
C	0. 06807900	1. 43365500	-5. 53667500
H	1. 50275400	0. 14289500	-4. 64377400
C	-0. 09146500	3. 68998300	-4. 68341900
C	1. 39308400	4. 39510600	-2. 84749500
C	-0. 52233300	2. 72888300	-5. 55834600
H	-0. 31069400	0. 66139200	-6. 19992600
H	-0. 53893300	4. 68192600	-4. 68066500
H	0. 90204300	5. 36665500	-2. 83604600
H	-1. 32108900	2. 94528900	-6. 26344600
C	1. 07731700	-3. 66963400	2. 15378900
C	0. 44172300	-2. 95098800	3. 19576100
C	0. 39317600	-4. 71911000	1. 49228800
C	1. 07500700	-1. 87362800	3. 89823300
C	-0. 90532500	-3. 30116500	3. 58576300
C	-0. 96087900	-5. 04399500	1. 87868100
C	0. 44359800	-1. 22005200	4. 92562300
H	2. 06986300	-1. 56459900	3. 60002000
C	-1. 52972900	-2. 59122100	4. 65970000
C	-1. 56981300	-4. 33119800	2. 91527600
C	-0. 87649800	-1. 58508700	5. 31792700
H	0. 95021200	-0. 40689900	5. 43796300
H	-2. 54046600	-2. 87607800	4. 94385500
H	-2. 58221100	-4. 59398500	3. 21614700
H	-1. 36029500	-1. 05707500	6. 13537400
C	4. 65485400	3. 71573800	-0. 27260800
H	5. 51544000	3. 56080200	0. 37278300
C	4. 26641800	2. 72525100	-1. 13622900
H	4. 82750900	1. 79918500	-1. 17248400
C	3. 94366400	4. 94705000	-0. 20828100
H	4. 24930700	5. 71389400	0. 49729100
C	2. 87626500	5. 15949500	-1. 03781400

H	2.32540700	6.09547000	-1.00225600
C	0.31171500	-6.52983000	-0.14780000
H	0.79572200	-7.11476500	-0.92533900
C	-1.02968900	-6.83069100	0.22209700
H	-1.55855200	-7.63768100	-0.27792300
C	-1.64241200	-6.10852200	1.20973600
H	-2.66267500	-6.33483600	1.51119300
C	0.99689500	-5.51451000	0.46618800
H	2.01997900	-5.30550900	0.17583000
N	0.67182000	-0.87031800	-1.84277500
S	-0.83423100	-1.26914400	-2.02354500
O	-1.51746300	-0.41438500	-3.01107300
O	-1.58484800	-1.51563000	-0.75523900
C	-0.80173200	-2.95151300	-2.83354300
F	-0.17585000	-2.87958200	-4.01338200
F	-2.06038100	-3.36615600	-3.03716900
F	-0.17230400	-3.83399000	-2.05730600
C	-5.06954700	0.04862800	-0.55580500
C	-4.37728000	0.83336600	-1.70808100
H	-5.01033700	0.79176000	-2.60972500
H	-3.47375800	0.29475200	-2.00601300
C	-4.01881300	2.27883200	-1.55669300
C	-4.27568900	0.28638800	0.77523900
H	-4.72137900	1.10103500	1.34122200
H	-4.33627600	-0.60821700	1.40021500
N	-2.85783300	0.62440400	0.61441900
C	-2.22576900	1.61557500	1.28286200
N	-0.88420400	1.52768800	1.36064500
C	0.01207500	2.44445500	1.98024400
C	0.02242100	3.81295400	1.69572600
C	0.96495200	1.90633100	2.84705900
C	0.96267300	4.63574600	2.31386400
C	1.90456700	2.74113600	3.45189300
H	0.97373500	0.83870400	3.02989400
C	1.90677200	4.11043000	3.19841700
H	2.64268200	4.75502300	3.66341200
C	2.88539400	2.13536300	4.42044000
C	0.93910500	6.11834400	2.05504800
F	2.29332100	1.84890700	5.60928300
F	3.39669500	0.97413100	3.95778000
F	3.91872900	2.96148800	4.68516300
F	0.21301700	6.77792900	2.98612200
F	2.18132300	6.65452900	2.07980400
F	0.39498800	6.41639300	0.85177900

S	-3.10472100	2.95438600	1.95106200
H	-0.68483700	4.23134900	0.99337500
H	-0.40958400	0.64641700	1.08106000
H	-2.27224600	-0.11408000	0.19493900
C	-4.70194700	3.16323900	-0.69911900
H	-5.67677200	2.80082600	-0.36597700
H	-4.04587300	2.99959200	0.36602200
C	-5.00649200	-1.46570700	-1.01621600
H	-3.95982700	-1.70518500	-1.23036700
H	-5.54350800	-1.51366100	-1.97081400
C	-6.55395100	0.42026900	-0.36011500
C	-7.16013700	0.40113600	0.90709200
C	-7.38426500	0.69807100	-1.45984800
C	-8.51882800	0.67833300	1.07187000
H	-6.57943700	0.15733800	1.78994900
C	-8.74240000	0.97449300	-1.30142600
H	-6.97960800	0.69577300	-2.46775100
C	-9.31836600	0.97208500	-0.03089200
H	-8.94921900	0.65793300	2.06954300
H	-9.34915800	1.19141400	-2.17669700
H	-10.37514800	1.18996400	0.09566900
C	-5.57138600	-2.52263600	-0.08095900
C	-6.84246200	-2.93150300	-0.22579900
H	-7.43961400	-2.46371100	-1.00906100
C	-2.86381100	2.76165400	-2.37442900
H	-2.16803700	3.34514800	-1.75656100
H	-2.31310300	1.94925500	-2.85112900
H	-3.22194700	3.45570300	-3.14869500
C	-4.62603000	-3.12304200	0.94608000
H	-3.58021100	-2.96471100	0.66564100
H	-4.76346400	-2.69561400	1.94984500
H	-4.77411300	-4.20355400	1.04593800
C	-4.63564600	4.67682300	-0.89305900
H	-5.20968100	4.98158600	-1.77604200
H	-5.06494300	5.18040100	-0.02211100
H	-3.61005900	5.03667200	-1.01215100
C	-7.56929700	-3.96668800	0.58413200
H	-8.41796000	-3.51461400	1.11654000
H	-7.99015900	-4.74860000	-0.06262800
H	-6.93254100	-4.45095300	1.32940700

TS-EF-6RR-2

l imaginary frequency

H = -5393.917506

G = -5394.125310

E(M06-2X-DCM) = -5394.846719

O	-2.27348700	-1.60313800	-1.04130500
O	-1.71862000	-1.76233900	1.49767100
P	-1.24316100	-1.04803100	0.10194400
O	-1.32941300	0.43241500	0.32703600
C	-6.44493700	-1.49235600	-0.64653000
C	-5.69563400	-2.46675100	0.00244600
C	-4.30546100	-2.54497600	-0.17787300
C	-4.39522500	-0.58560300	-1.63511100
C	-5.79396000	-0.58805200	-1.48106600
C	-1.51777500	-3.13656100	1.65476600
C	-2.38946700	-4.03136600	1.03932400
C	-2.06048100	-5.39596400	1.00702100
C	-0.95583500	-5.87436500	1.70198800
C	-0.18280900	-4.97835400	2.44010300
C	-0.43001900	-3.59551600	2.42234300
H	-6.37149400	0.15078400	-2.02813500
H	0.65532700	-5.34305000	3.02635400
C	-3.78177100	-3.83529500	0.44910800
C	-4.86533800	-4.06090600	1.55983600
H	-4.60644200	-3.44692800	2.43033500
H	-4.91322600	-5.10252300	1.89054000
H	-3.71242600	-6.78396500	0.75250600
H	-2.54070600	-6.83121200	-0.56030200
C	-3.65935000	-1.56222300	-0.93076400
H	-7.52363400	-1.44313000	-0.52121100
H	-0.70142700	-6.93108900	1.68585000
C	-6.17971100	-3.55157600	0.93732900
H	-6.88772100	-3.17650300	1.68533800
H	-6.69786000	-4.34812400	0.38501000
C	-3.04321300	-6.15917300	0.14469400
C	-3.81578700	-5.02552800	-0.56654000
H	-3.27570000	-4.72667200	-1.47137900
H	-4.83429000	-5.30453700	-0.85437400
C	0.42726700	-2.69757600	3.25729700
C	1.81354100	-2.58831900	2.98682100
C	-0.12700800	-2.06173100	4.39786300
C	2.42563600	-3.17656800	1.83232700
C	2.66368800	-1.85022600	3.89499100
C	0.72988400	-1.29655800	5.27588200
C	3.77603300	-3.08396700	1.61913000
H	1.80052100	-3.67561600	1.10321800
C	4.07035200	-1.78940800	3.64099400

C	2.09885200	-1.21812300	5.00530500
C	4.61679100	-2.39897000	2.54318100
H	4.20654600	-3.52042300	0.72298500
H	4.69760900	-1.24861600	4.34634700
H	2.74267100	-0.66161500	5.68388900
H	5.68472300	-2.34176700	2.35598600
C	-3.80195300	0.41219800	-2.58036900
C	-4.02308000	1.79743100	-2.36028200
C	-3.15637200	-0.02122400	-3.76733700
C	-4.64481700	2.30983600	-1.17442400
C	-3.62193700	2.75716200	-3.36562900
C	-2.72060200	0.95427000	-4.74228500
C	-4.90450500	3.64778500	-1.01866600
H	-4.91013500	1.61803600	-0.38393100
C	-3.90733100	4.14525500	-3.16401400
C	-2.97591200	2.31104200	-4.52262300
C	-4.54352600	4.58199400	-2.03195100
H	-5.38796600	4.00098300	-0.11181700
H	-3.61897600	4.84692800	-3.94382100
H	-2.68333000	3.03515600	-5.28118200
H	-4.77470600	5.63623200	-1.90237300
C	-2.01088400	-1.55134400	5.87324800
H	-3.06416100	-1.65525800	6.12024000
C	-1.50947700	-2.16911000	4.75716500
H	-2.16770800	-2.76259800	4.13342400
C	-1.16571600	-0.77918000	6.72018600
H	-1.57995300	-0.29790100	7.60219600
C	0.16587600	-0.66064500	6.42638900
H	0.82765700	-0.08676800	7.07120100
C	-2.31137000	-1.78531800	-5.23139800
H	-2.14795900	-2.84095600	-5.42805200
C	-1.85810800	-0.81859200	-6.17165800
H	-1.35372700	-1.14318200	-7.07750300
C	-2.06550200	0.51224800	-5.93376800
H	-1.73843500	1.26278800	-6.64959500
C	-2.94342500	-1.40135500	-4.07890800
H	-3.28429100	-2.15679000	-3.38345700
N	0.20214800	-1.66736800	-0.26998700
S	0.83023900	-1.94882100	-1.70657500
O	2.27473100	-2.16703700	-1.53662400
O	0.38750100	-1.03051900	-2.77156300
C	0.21760400	-3.65014500	-2.21662000
F	0.37954000	-4.51843900	-1.20866800
F	0.92976300	-4.06976600	-3.26694700

F	-1.07909700	-3.64090700	-2.56230600
C	-0.84215800	3.90005100	1.03617200
C	-0.97138300	3.57613100	-0.48606200
H	-1.79457100	4.16644100	-0.91614100
H	-1.30406200	2.53956800	-0.58333900
C	0.18660600	3.77875800	-1.41812600
C	0.45649300	3.23138000	1.59783700
H	1.27849400	3.94219700	1.60586000
H	0.28816900	2.92735800	2.63475800
N	0.93905500	2.06836100	0.84551800
C	2.21781400	1.89225200	0.46058700
N	2.60083700	0.65833600	0.06856000
C	3.88642900	0.37952700	-0.50928700
C	4.00308700	0.21726800	-1.88895800
C	5.00396100	0.26460300	0.31466600
C	5.25620100	-0.04176000	-2.44478900
C	6.25276400	0.00482200	-0.25190900
H	4.89645100	0.37932300	1.38618000
C	6.38502500	-0.14433300	-1.63216800
H	7.35878300	-0.32748200	-2.07126100
C	7.45603300	-0.16554800	0.63595400
C	5.38703400	-0.25273800	-3.93108900
F	7.62545400	-1.46208200	1.00531500
F	8.59537900	0.21080900	0.01749400
F	7.35000400	0.55146400	1.77443800
F	4.44881500	0.43530200	-4.61772000
F	6.59759800	0.15093700	-4.38298700
F	5.25555700	-1.55213000	-4.26807100
S	3.33731200	3.21621600	0.37672000
H	3.12463600	0.28583800	-2.51854300
H	1.94445500	-0.12602500	0.13829300
H	0.26313200	1.29523600	0.72814100
C	1.17242500	4.76495800	-1.21546100
H	0.88882400	5.52751700	-0.48729600
H	1.99619700	4.10893900	-0.51943900
C	0.22767500	2.84709900	-2.58233200
H	-0.69676700	2.97230600	-3.16623100
H	1.07897200	3.00600500	-3.24437400
H	0.20745800	1.79912100	-2.25597700
C	-0.83138800	5.41505400	1.33557500
C	-1.68561900	6.28940800	0.63949500
C	-0.05163900	5.97001200	2.36379800
C	-1.73499900	7.65192700	0.93268700
H	-2.33719100	5.91073600	-0.14266000

C	-0.09730400	7.33437500	2.66072700
H	0.59598700	5.34118200	2.96405400
C	-0.93493500	8.18582800	1.94382200
H	-2.40323300	8.29642500	0.36728100
H	0.52420400	7.72544000	3.46190300
H	-0.96983600	9.24746400	2.17207200
C	-2.14169200	3.28115100	1.69858200
H	-2.24920200	2.26275300	1.31499300
H	-2.98942200	3.85517500	1.30960300
C	-2.20468300	3.23377900	3.22037600
C	-2.58034700	4.31586500	3.92335400
H	-2.81846400	5.21964800	3.36263600
C	-1.92606600	1.87808600	3.83168100
H	-2.72018300	1.16953100	3.55987500
H	-1.00092300	1.43069200	3.45002600
H	-1.85778000	1.89694400	4.92133900
C	-2.73609500	4.45786300	5.41171400
H	-2.13297700	5.29666500	5.78539800
H	-3.77867200	4.68609700	5.67473900
H	-2.44346100	3.56237200	5.96561200
C	2.05907400	5.29855700	-2.34106600
H	1.47786300	5.90488600	-3.04479600
H	2.83980400	5.93490600	-1.91410200
H	2.55680400	4.50210800	-2.89987300

TS-1-1-6SS

l imaginary frequency

H = -5393.912882

G = -5394.117237

E(M06-2X-DCM) = -5394.839246

C	2.76908300	3.39139400	1.92446900
C	1.59218000	3.16315800	2.93655400
H	2.02953800	3.20004300	3.94537100
H	0.93183600	4.03060100	2.84485100
C	0.72932600	1.91803300	2.93859700
C	2.16008700	3.70460700	0.52849200
H	2.91245400	3.57560300	-0.25507700
H	1.87312100	4.75549900	0.51437100
N	0.95867900	2.96312200	0.17612100
C	-0.22424500	3.56149800	-0.17783500
N	-1.11028300	2.65518300	-0.70296900
C	-2.41781600	2.77771800	-1.19492200
C	-3.32358000	3.79851100	-0.86759000
C	-2.84334000	1.74012300	-2.04228200

C	-4.61449700	3.76858600	-1.39567200
C	-4.13441700	1.73198500	-2.56155000
H	-2.15591400	0.93807000	-2.29227200
C	-5.03548700	2.74982800	-2.25040400
H	-6.03680400	2.75065300	-2.66347100
C	-4.57694200	0.56422700	-3.39792700
C	-5.61192400	4.80994000	-0.95917400
F	-3.58030500	0.09243200	-4.18397200
F	-5.61709300	0.86865600	-4.19807600
F	-4.97445000	-0.48127400	-2.61913700
F	-5.02456500	5.96657000	-0.59881200
F	-6.32954500	4.38051400	0.11296000
F	-6.50609000	5.08853100	-1.93341600
S	-0.53728200	5.20793700	0.04095600
H	-3.01614700	4.60303700	-0.21576000
C	1.20044100	0.64055100	3.26765000
H	-0.75153100	1.69807600	-0.76434700
H	1.06671700	1.98416600	-0.08667500
H	1.16901700	-0.20578900	2.19774400
O	-1.36288800	-1.59604700	0.14505500
O	0.86735200	-2.24066900	-1.06376900
P	0.20571600	-1.18722200	-0.01555200
O	0.22215100	0.22999000	-0.48440100
C	-2.76865100	-5.47841400	0.92368200
C	-2.20732600	-5.16452000	-0.30723800
C	-1.83815700	-3.84461200	-0.61302300
C	-2.53245900	-3.14006200	1.61880400
C	-2.97468300	-4.45673400	1.84482700
C	0.48024700	-2.13218600	-2.41670500
C	-0.71722700	-2.72018700	-2.81476000
C	-1.20697500	-2.47326900	-4.10811500
C	-0.46110100	-1.73555900	-5.01947400
C	0.79040000	-1.25871800	-4.63599800
C	1.28862200	-1.43082700	-3.33246300
H	-3.47781500	-4.67161800	2.78192700
H	1.40525000	-0.71871100	-5.34975600
C	-1.60564300	-3.74028500	-2.11817400
C	-1.11814000	-5.19457700	-2.42789200
H	-1.23491600	-5.45714300	-3.48379700
H	-0.05343200	-5.26803900	-2.17798700
H	-3.27980700	-2.41433100	-4.76253200
H	-2.50810800	-3.99042000	-4.94142500
C	-1.89034700	-2.87553300	0.38985800
H	-3.07463100	-6.49534200	1.15520700

H	-0.83637600	-1.54470400	-6.02142600
C	-1.94197000	-6.08632100	-1.47670700
H	-2.87885500	-6.41823500	-1.94505300
H	-1.40332200	-6.99218000	-1.17587900
C	-2.56816900	-3.10288500	-4.29640900
C	-2.96492700	-3.47332100	-2.85299000
H	-3.64410100	-4.32861000	-2.79257300
H	-3.46389900	-2.61833400	-2.38451900
C	2.66566200	-0.91681000	-3.04744400
C	3.74150300	-1.83213300	-2.93625600
C	2.91517500	0.47706800	-3.05972900
C	3.56287000	-3.25184100	-2.98028500
C	5.09259100	-1.33319700	-2.80918000
C	4.27389200	0.96155200	-2.95845800
C	4.62609900	-4.10964800	-2.87320100
H	2.56252100	-3.65112100	-3.10071100
C	6.17382100	-2.26236100	-2.69289700
C	5.32182100	0.04585200	-2.82802600
C	5.95128600	-3.61237300	-2.71986500
H	4.45867700	-5.18269900	-2.90630300
H	7.18196300	-1.86764900	-2.59034400
H	6.34275200	0.41517000	-2.75351700
H	6.78115400	-4.30828700	-2.63323000
C	-2.85475200	-2.11922900	2.66391300
C	-3.70284000	-1.02282300	2.35164100
C	-2.44354400	-2.33641500	4.00657600
C	-4.23057800	-0.78602800	1.04166900
C	-4.10840700	-0.11067600	3.39931600
C	-2.91337300	-1.45237100	5.05096000
C	-5.03151100	0.29309500	0.77443400
H	-4.00087900	-1.48255300	0.24484500
C	-4.92604400	1.01783800	3.07297600
C	-3.71706700	-0.35944100	4.71767200
C	-5.36785500	1.22674200	1.79485400
H	-5.41460000	0.43375800	-0.23030000
H	-5.19431600	1.70463500	3.87252400
H	-4.05351800	0.31171300	5.50575700
H	-5.97040900	2.09645400	1.54910300
C	2.14717300	2.79347200	-3.22573600
H	1.33590600	3.51026500	-3.31690500
C	1.87101200	1.45125000	-3.18067400
H	0.84445700	1.10883600	-3.22992300
C	3.49013400	3.26330900	-3.14336500
H	3.68949600	4.33046400	-3.18529300

C	4. 51911000	2. 37038000	-3. 00580100
H	5. 54782300	2. 71557300	-2. 93469300
C	-1. 19210200	-3. 58390700	5. 69786400
H	-0. 50206600	-4. 38350200	5. 95264700
C	-1. 69877200	-2. 74020400	6. 72665900
H	-1. 41149700	-2. 91660800	7. 75972500
C	-2. 52715000	-1. 69924300	6. 40607200
H	-2. 90629800	-1. 03232500	7. 17710800
C	-1. 54790900	-3. 38977900	4. 38794200
H	-1. 11811000	-4. 01963300	3. 61892400
N	1. 08673000	-1. 35921900	1. 37114200
S	1. 71341000	-2. 75474900	1. 98176300
C	3. 13724300	-3. 24479200	0. 83164700
O	0. 77629200	-3. 87818300	1. 89940400
O	2. 36782300	-2. 41270400	3. 24449200
F	2. 72223500	-4. 14646000	-0. 05539500
F	3. 62443700	-2. 17889500	0. 19518300
F	4. 09897200	-3. 78570000	1. 58278100
C	3. 76987600	2. 22521800	1. 96236900
C	4. 45444700	1. 93913200	3. 15922300
C	4. 06127600	1. 42889600	0. 84874900
C	5. 39263700	0. 91320900	3. 23734100
H	4. 25352600	2. 52404700	4. 05313800
C	5. 01227400	0. 40545900	0. 91833200
H	3. 56029200	1. 59563000	-0. 09844600
C	5. 68165500	0. 14171900	2. 10989700
H	5. 89818900	0. 71748200	4. 17928400
H	5. 21623400	-0. 18719600	0. 03350600
H	6. 41372900	-0. 65902500	2. 16454300
C	3. 46873400	4. 72409000	2. 40333300
H	2. 66773300	5. 44716500	2. 59633800
H	3. 95319100	4. 53019600	3. 36874000
C	4. 47689500	5. 36981900	1. 46534800
C	4. 14152000	6. 51039400	0. 83711200
H	3. 14141200	6. 90639700	1. 01990300
C	0. 30647600	-0. 21746400	4. 18066700
H	-0. 66214200	-0. 43422100	3. 73206700
H	0. 80343200	-1. 16366500	4. 38897500
H	0. 13002700	0. 30063800	5. 13167500
C	4. 96279600	7. 34060600	-0. 10854600
H	4. 46584600	7. 41537700	-1. 08559300
H	5. 06447900	8. 36863500	0. 26511100
H	5. 96741200	6. 94463900	-0. 27728400
C	5. 83128200	4. 70886300	1. 34920300

H	6.55430000	5.33239000	0.81807500
H	6.24244200	4.49362800	2.34393900
H	5.77229300	3.74605500	0.82885600
H	2.26161500	0.58721000	3.50964400
C	-0.74864400	2.15695800	2.86339700
H	-0.99491900	3.07905200	2.33444600
H	-1.28611800	1.31567500	2.41722600
H	-1.13264800	2.25235300	3.89196500

TS-1-1-6SS-1

l imaginary frequency

H = -5393.910600

G = -5394.115144

E(M06-2X-DCM) = -5394.837522

C	2.89933900	3.35222600	1.74869000
C	1.74054200	3.22178200	2.79643400
H	2.20246800	3.25121400	3.79378800
H	1.13392900	4.12771900	2.70286200
C	0.80386900	2.03196000	2.84135700
C	2.25725900	3.63970700	0.36150900
H	2.97295900	3.44545800	-0.44178200
H	2.00582300	4.69927300	0.32008100
N	1.01564800	2.93683200	0.07343700
C	-0.14861700	3.57503900	-0.27929200
N	-1.08222900	2.69195100	-0.75602800
C	-2.40055400	2.84952800	-1.20773000
C	-3.26081400	3.90572400	-0.87111500
C	-2.88828300	1.80862100	-2.01653600
C	-4.57107200	3.90476400	-1.35041700
C	-4.19713700	1.83011800	-2.48855600
H	-2.23537500	0.98007200	-2.27245500
C	-5.05448200	2.88182300	-2.16644800
H	-6.07030300	2.90518500	-2.54168600
C	-4.70446800	0.65908700	-3.28295100
C	-5.51987400	4.98407200	-0.89794700
F	-3.75377500	0.14615700	-4.09953100
F	-5.76848800	0.97657200	-4.04564300
F	-5.09613500	-0.36070600	-2.46810800
F	-4.88559200	6.13118000	-0.59020400
F	-6.20241600	4.59966200	0.21332600
F	-6.44646600	5.26616600	-1.84022800
S	-0.38627100	5.23966100	-0.11108100
H	-2.90489000	4.71390500	-0.24898900
C	1.20693100	0.73445900	3.18432600

H	-0.76142400	1.72046600	-0.80434200
H	1.08047800	1.94910000	-0.17170500
H	1.14613300	-0.13213400	2.13360500
O	-1.44500100	-1.54431700	0.18649300
O	0.74040500	-2.26368700	-1.06218000
P	0.12493300	-1.16869600	-0.02795000
O	0.15435900	0.23184300	-0.54411500
C	-2.91532200	-5.38007800	1.07142800
C	-2.38209300	-5.09930700	-0.17983000
C	-1.98918000	-3.79402000	-0.51684800
C	-2.60147400	-3.03777400	1.72242600
C	-3.06847500	-4.33983700	1.98186200
C	0.32350200	-2.17069700	-2.40815700
C	-0.89828700	-2.73463200	-2.76569000
C	-1.41558600	-2.49625900	-4.04991900
C	-0.67463800	-1.79493800	-4.99331000
C	0.59738300	-1.34301200	-4.64978400
C	1.12382900	-1.50280300	-3.35564400
H	-3.54849200	-4.52809100	2.93660600
H	1.20635300	-0.83017700	-5.38814100
C	-1.79563100	-3.71843800	-2.02917200
C	-1.35683000	-5.19005400	-2.33021400
H	-1.51188700	-5.46467900	-3.37807800
H	-0.28747500	-5.28898400	-2.11092700
H	-3.50288400	-2.38635400	-4.64847900
H	-2.78327600	-3.98744600	-4.82259300
C	-1.99072600	-2.80778600	0.47065700
H	-3.24006700	-6.38520100	1.32764400
H	-1.07053100	-1.61187800	-5.98877100
C	-2.17541100	-6.04514100	-1.34179500
H	-3.13420800	-6.35854500	-1.77743700
H	-1.65235100	-6.96068300	-1.04275800
C	-2.79910200	-3.08862200	-4.19076700
C	-3.16648300	-3.42419500	-2.73110100
H	-3.86764800	-4.25856600	-2.63793400
H	-3.62793800	-2.54775100	-2.26364800
C	2.51602500	-1.00735400	-3.11485900
C	3.57846500	-1.93797500	-3.00154000
C	2.78946500	0.38105600	-3.17589500
C	3.37429800	-3.35482300	-2.99724400
C	4.94074200	-1.45982400	-2.92397700
C	4.15866300	0.84351600	-3.12604800
C	4.42491500	-4.22801100	-2.89003500
H	2.36444300	-3.73945100	-3.07997600

C	6.00842300	-2.40431700	-2.80609600
C	5.19359400	-0.08652400	-2.99329000
C	5.76193700	-3.75029500	-2.78537200
H	4.23816000	-5.29835300	-2.88530700
H	7.02556500	-2.02494400	-2.74148800
H	6.22249800	0.26612900	-2.95828800
H	6.58160400	-4.45809900	-2.69796900
C	-2.86615400	-1.99566500	2.76276400
C	-3.69035700	-0.87839800	2.46078100
C	-2.42352500	-2.20909900	4.09630500
C	-4.24598400	-0.63948700	1.16268800
C	-4.04052300	0.05660800	3.50844000
C	-2.84199800	-1.30259700	5.14308400
C	-5.01913300	0.46174800	0.90393700
H	-4.05998000	-1.35148200	0.36819500
C	-4.83074300	1.20703100	3.19053600
C	-3.62345000	-0.19087600	4.81902300
C	-5.29844400	1.41681000	1.92180700
H	-5.42445100	0.60347100	-0.09184300
H	-5.05665000	1.91006800	3.98907500
H	-3.91954900	0.49778800	5.60818600
H	-5.87924700	2.30280700	1.68154700
C	2.05812400	2.70508900	-3.39736100
H	1.25736500	3.43346000	-3.48960700
C	1.75984000	1.37050500	-3.29927600
H	0.72635500	1.04619800	-3.30770500
C	3.41118900	3.15210100	-3.37013000
H	3.62856400	4.21293800	-3.46033300
C	4.42767200	2.24522600	-3.22903400
H	5.46401200	2.57306800	-3.19882600
C	-1.15699100	-3.46917700	5.76702900
H	-0.47925100	-4.28234000	6.01163600
C	-1.61545100	-2.60339900	6.79987200
H	-1.30478600	-2.77629300	7.82673900
C	-2.42634600	-1.54552900	6.49012500
H	-2.76776800	-0.86125200	7.26357200
C	-1.54360000	-3.27986400	4.46505300
H	-1.14986400	-3.92772900	3.69182400
N	1.03479300	-1.30792600	1.34271700
S	1.65722700	-2.69147500	1.98279500
C	3.06366600	-3.21544000	0.82563300
O	0.71130900	-3.80960000	1.93689000
O	2.32540100	-2.32258300	3.23058500
F	2.63539200	-4.15128900	-0.01881400

F	3.53077600	-2.17181200	0.13977400
F	4.04361700	-3.72285400	1.57655700
C	3.85591900	2.15006900	1.80255100
C	4.49816800	1.83397600	3.01553600
C	4.16830300	1.36444400	0.68848300
C	5.40758000	0.78410700	3.11084400
H	4.28666700	2.41507500	3.90970700
C	5.08965600	0.31544300	0.77535300
H	3.70333900	1.55347700	-0.27245800
C	5.71209200	0.01802500	1.98362200
H	5.87705400	0.56428000	4.06604900
H	5.30487200	-0.27242900	-0.11043600
H	6.41949700	-0.80363600	2.05182500
C	3.69615900	4.65014800	2.17201900
H	2.96601200	5.46903300	2.23417100
H	4.06799200	4.48965700	3.18876000
C	4.86417000	5.08853000	1.29937900
C	6.11547400	4.76935400	1.67027300
H	6.23342700	4.18312700	2.58162300
C	0.27340700	-0.06331000	4.11043200
H	-0.70709700	-0.23364400	3.66717700
H	0.72023000	-1.03205100	4.32974100
H	0.12723700	0.47339600	5.05627700
C	7.40788900	5.09318400	0.97642700
H	8.09682100	5.61334200	1.65579300
H	7.91702300	4.17039200	0.66528400
H	7.28010200	5.71414800	0.08601500
C	4.54708500	5.92439600	0.07668600
H	5.40861600	6.50900800	-0.25609200
H	4.22347700	5.31351800	-0.77579400
H	3.73170000	6.62791900	0.28454500
H	2.26584000	0.62796900	3.41974000
C	-0.65859800	2.35896900	2.80131800
H	-0.86336900	3.28779000	2.26652600
H	-1.25816900	1.54631900	2.38205700
H	-1.00688300	2.48986300	3.83873400

TS-1-1-6SS-2

l imaginary frequency

H = -5393.910192

G = -5394.114919

E(M06-2X-DCM) = -5394.835677

C	0.94931300	4.63647300	0.69930200
C	-0.02945500	4.23421000	1.85081300

H	0.36446400	4.67467300	2.77679400
H	-0.97754200	4.73891300	1.64833700
C	-0.32363100	2.78806500	2.18798500
C	0.28268900	4.31760500	-0.66495100
H	1.01920600	4.41099300	-1.47166000
H	-0.48523800	5.06283500	-0.85299800
N	-0.39948300	3.03548800	-0.76221800
C	-1.68108300	2.89674700	-1.23498500
N	-2.01801400	1.58059800	-1.41417800
C	-3.19872800	0.95602000	-1.84474600
C	-4.49021300	1.49472400	-1.73990400
C	-3.04540600	-0.34360600	-2.35649300
C	-5.58718100	0.74000800	-2.15576500
C	-4.15327900	-1.07858400	-2.76886800
H	-2.05257800	-0.77637500	-2.42821900
C	-5.43805600	-0.54373100	-2.68064200
H	-6.29941000	-1.11051100	-3.01247500
C	-3.95862500	-2.49463600	-3.23364000
C	-6.97637800	1.28310700	-1.94397200
F	-2.80592600	-2.65081600	-3.92637800
F	-4.96667000	-2.92169400	-4.01889900
F	-3.89009200	-3.35697200	-2.18053200
F	-7.00883900	2.62916400	-1.94759400
F	-7.48230500	0.87935100	-0.74809200
F	-7.83584900	0.84808700	-2.89157700
S	-2.71365600	4.20113700	-1.53590600
H	-4.62926800	2.48984100	-1.34378400
C	0.59491000	1.94019100	2.82205600
H	-1.26696100	0.91425300	-1.20965200
H	0.16878300	2.18935900	-0.73755300
H	1.04978600	0.95376600	2.00524400
O	-0.38963400	-1.94577900	0.58015800
O	1.95805800	-1.78547000	-0.56735700
P	0.81852200	-0.91838400	0.20631100
O	0.21060800	0.16293400	-0.62441000
C	0.10647600	-5.67244000	2.45880700
C	0.54089200	-5.47519300	1.15458200
C	0.27796300	-4.26929800	0.48515100
C	-0.81181300	-3.39948800	2.48814400
C	-0.61038500	-4.65825300	3.08481800
C	1.64826400	-2.23485100	-1.86947800
C	0.88308200	-3.38992900	-2.00984700
C	0.41147800	-3.75255100	-3.28244700
C	0.78265100	-3.02824700	-4.40857500

C	1. 64894300	-1. 94838500	-4. 25765900
C	2. 09574800	-1. 51699100	-2. 99566200
H	-1. 02112200	-4. 82394300	4. 07534300
H	1. 98675100	-1. 40049000	-5. 13209200
C	0. 52747400	-4. 47636600	-1. 00594300
C	1. 64925900	-5. 56593700	-0. 95484800
H	1. 73007200	-6. 12487700	-1. 89215800
H	2. 61056300	-5. 07147400	-0. 77355800
H	-1. 40947100	-4. 83299000	-3. 77631000
H	0. 01314400	-5. 85879200	-3. 58784000
C	-0. 28197300	-3. 20558600	1. 19394100
H	0. 28878600	-6. 61272800	2. 97261700
H	0. 42005200	-3. 30622000	-5. 39466100
C	1. 27570700	-6. 44507200	0. 25616800
H	0. 63084200	-7. 28458300	-0. 03810400
H	2. 15331200	-6. 88078400	0. 74733400
C	-0. 48959200	-4. 96294400	-3. 19779800
C	-0. 75517500	-5. 07261300	-1. 68307700
H	-0. 96499300	-6. 09271000	-1. 34868300
H	-1. 61904700	-4. 45199000	-1. 42209300
C	3. 07235900	-0. 38190700	-2. 97537900
C	4. 44058200	-0. 64486300	-2. 71612000
C	2. 66315100	0. 90531700	-3. 40110500
C	4. 92482100	-1. 93300800	-2. 32135800
C	5. 41468400	0. 40964800	-2. 88951700
C	3. 65059900	1. 94423700	-3. 59136900
C	6. 25606900	-2. 15406300	-2. 08336000
H	4. 21843300	-2. 74689800	-2. 20751000
C	6. 79448300	0. 13796900	-2. 62814800
C	4. 99601400	1. 66848200	-3. 33134000
C	7. 20718600	-1. 10519200	-2. 23207400
H	6. 59266000	-3. 14129900	-1. 77901800
H	7. 51088600	0. 94581200	-2. 75779700
H	5. 73679800	2. 45131400	-3. 48206800
H	8. 25826800	-1. 29944800	-2. 03718600
C	-1. 64043200	-2. 40907200	3. 24287500
C	-2. 86704900	-1. 94233300	2. 69835000
C	-1. 27703300	-2. 05912200	4. 57157400
C	-3. 34540000	-2. 31899200	1. 40214900
C	-3. 71826300	-1. 07880200	3. 48825100
C	-2. 17510800	-1. 25482900	5. 37086900
C	-4. 52244400	-1. 82909400	0. 90035000
H	-2. 76879900	-3. 01664800	0. 80766700
C	-4. 92857400	-0. 57010900	2. 91776600

C	-3.35884500	-0.77569000	4.80423800
C	-5.31819400	-0.92041400	1.65365000
H	-4.85057700	-2.14236400	-0.08477000
H	-5.53710700	0.10002300	3.52075000
H	-4.02110900	-0.15466500	5.40462400
H	-6.22647000	-0.51408800	1.21794400
C	0.93051600	2.48187900	-4.10546400
H	-0.11551100	2.70571500	-4.29525400
C	1.29398900	1.23459700	-3.66681000
H	0.53710000	0.47702300	-3.50356400
C	1.91127100	3.49589700	-4.30819900
H	1.60505000	4.47576900	-4.66407900
C	3.23031400	3.23215000	-4.05167100
H	3.98799000	3.99878000	-4.19563300
C	0.27546600	-2.10851400	6.46122400
H	1.23413800	-2.40357500	6.87874900
C	-0.63777500	-1.36322600	7.25941600
H	-0.38104500	-1.11722900	8.28627900
C	-1.82310700	-0.94109300	6.72142000
H	-2.52213000	-0.35099000	7.30979700
C	-0.02955000	-2.44216600	5.16651100
H	0.69872800	-2.97331100	4.56623300
N	1.58181100	-0.28055200	1.52301400
S	2.72797000	-1.00226300	2.45737100
C	4.29658200	-1.07848200	1.39551100
O	2.42038800	-2.40493300	2.75016600
O	3.05084300	-0.06486900	3.53324100
F	4.40949400	-2.28001200	0.83205700
F	4.28024900	-0.14044300	0.44927100
F	5.34315300	-0.87542800	2.19929900
C	2.34658700	4.01789500	0.89800800
C	3.04159600	4.25092800	2.10085100
C	3.00792800	3.28364000	-0.09242700
C	4.33136400	3.77026700	2.30766200
H	2.57055900	4.81885500	2.89927800
C	4.30800900	2.80775400	0.10617500
H	2.52735200	3.06907500	-1.04041300
C	4.97525500	3.04499100	1.30370700
H	4.83149000	3.96205000	3.25314800
H	4.78750400	2.23869100	-0.68236400
H	5.98049900	2.66343400	1.45869600
C	1.16804200	6.20555000	0.75174700
H	1.80593500	6.40867400	1.61544600
H	1.77289700	6.45631100	-0.13069700

C	-0.03372000	7.13960100	0.82642900
C	-0.41375600	7.60853200	2.02845100
H	0.15695400	7.28065700	2.89972400
C	0.04996800	1.00917900	3.91675700
H	-0.69233800	0.30906000	3.53500200
H	0.86968900	0.43551200	4.34753700
H	-0.41873600	1.59557900	4.71695000
C	-1.54433200	8.54490200	2.34861900
H	-2.27414400	8.05897500	3.01099700
H	-1.17921200	9.43057800	2.88639700
H	-2.08477100	8.88517100	1.46201200
C	-0.69184900	7.56503000	-0.47085000
H	-1.15989500	8.54984900	-0.38667600
H	0.04823600	7.62228600	-1.27806700
H	-1.47008000	6.86451300	-0.79999700
H	1.55356800	2.39916100	3.06414200
C	-1.75954600	2.37090300	2.08657600
H	-2.31761100	2.96959100	1.36512600
H	-1.87137700	1.30781500	1.85541100
H	-2.22645100	2.51793800	3.07404800

TS-1-1-6SS-3

l imaginary frequency

H = -5393.910109

G = -5394.114614

E(M06-2X-DCM) = -5394.836875

C	0.86879900	4.57484000	1.13540500
C	-0.08330400	4.04084300	2.25618800
H	0.30731900	4.40431700	3.21607500
H	-1.05100200	4.52409500	2.09689300
C	-0.33172000	2.56117300	2.46598200
C	0.17538100	4.36631800	-0.23590900
H	0.88855100	4.55202700	-1.04818900
H	-0.61231800	5.11361000	-0.32447500
N	-0.48068400	3.08300300	-0.43409800
C	-1.76505000	2.95861700	-0.90745500
N	-2.07553700	1.65405200	-1.19362400
C	-3.24707800	1.04399600	-1.66657700
C	-4.54816900	1.54293900	-1.50024200
C	-3.07329400	-0.20133800	-2.29375500
C	-5.63441000	0.80439800	-1.96973500
C	-4.17088700	-0.92058000	-2.75827500
H	-2.07264900	-0.60431700	-2.41408200
C	-5.46530100	-0.42396100	-2.60884900

H	-6.31879300	-0.97769000	-2.98060500
C	-3.95278600	-2.28478800	-3.34997600
C	-7.03163800	1.29534600	-1.69389100
F	-2.80707800	-2.35286900	-4.06816300
F	-4.96263700	-2.66306400	-4.15771100
F	-3.85070000	-3.23583300	-2.37905800
F	-7.09317400	2.63549000	-1.57884700
F	-7.51151200	0.77719000	-0.53171500
F	-7.89542800	0.92561000	-2.66507400
S	-2.82416200	4.26141300	-1.08868100
H	-4.70204500	2.49577900	-1.01545800
C	0.62411400	1.68742100	3.00249500
H	-1.30698000	0.99013000	-1.05862100
H	0.10703600	2.25254500	-0.49854000
H	1.07819300	0.78683600	2.09592900
O	-0.33778300	-1.99997200	0.43657600
O	1.98504800	-1.68918400	-0.73050900
P	0.84504100	-0.91923400	0.13891100
O	0.20171900	0.22204100	-0.57679200
C	0.26139700	-5.86745300	1.96777700
C	0.66991300	-5.54633200	0.67989400
C	0.37182400	-4.29175600	0.12424200
C	-0.69952800	-3.62545600	2.21345200
C	-0.46418400	-4.92783400	2.69248900
C	1.65866300	-2.02685300	-2.06176700
C	0.91568100	-3.18196200	-2.29193100
C	0.42892600	-3.44048100	-3.58408800
C	0.76287400	-2.60974000	-4.64661400
C	1.60768400	-1.52728200	-4.41397800
C	2.06891900	-1.20066200	-3.12607800
H	-0.85450500	-5.18911800	3.67060100
H	1.91653400	-0.89532400	-5.24114000
C	0.60097500	-4.36068500	-1.38292500
C	1.74651300	-5.42456400	-1.44438100
H	1.82525100	-5.89600700	-2.42878200
H	2.69946400	-4.92628600	-1.23205000
H	-1.37556200	-4.51621300	-4.14436300
H	0.07282700	-5.52022200	-4.06941800
C	-0.19598600	-3.30686800	0.93350700
H	0.47087200	-6.84547300	2.39319100
H	0.38799900	-2.80701800	-5.64744300
C	1.41023900	-6.41616100	-0.31176700
H	0.77833900	-7.24008600	-0.67108900
H	2.30424800	-6.87446100	0.12638300

C	-0.44316800	-4.67473500	-3.59369100
C	-0.67984700	-4.92437700	-2.09088100
H	-0.86161500	-5.97468200	-1.84542200
H	-1.55234600	-4.34960000	-1.76255000
C	3.02090500	-0.04977200	-3.01805600
C	4.39916100	-0.30400900	-2.80801300
C	2.57586400	1.26167800	-3.31390300
C	4.91870500	-1.61214000	-2.54615100
C	5.34659100	0.78480800	-2.89609600
C	3.53682000	2.33665000	-3.42164800
C	6.25869100	-1.82348000	-2.35236200
H	4.23253100	-2.44963600	-2.49925500
C	6.73653600	0.52211100	-2.68396500
C	4.89241700	2.06946200	-3.20997000
C	7.18364600	-0.74303500	-2.41534700
H	6.62240800	-2.82704500	-2.14956100
H	7.43257900	1.35526800	-2.74751000
H	5.61297800	2.88026400	-3.29774200
H	8.24215000	-0.93008700	-2.25698400
C	-1.53276400	-2.72237000	3.06641700
C	-2.77768400	-2.23425300	2.58574300
C	-1.15205800	-2.48425900	4.41482000
C	-3.27215100	-2.50368700	1.26902400
C	-3.63076700	-1.46211000	3.46341200
C	-2.05058400	-1.77276900	5.29730300
C	-4.46734800	-1.99555400	0.83247900
H	-2.69316300	-3.13314300	0.60485300
C	-4.86080900	-0.92985100	2.96065700
C	-3.25333000	-1.26973800	4.79515500
C	-5.26663200	-1.17431900	1.67688000
H	-4.80727800	-2.22646700	-0.17118800
H	-5.47094600	-0.32876000	3.63103500
H	-3.91647500	-0.71857300	5.45939200
H	-6.19025800	-0.74975700	1.29400700
C	0.79661100	2.85625300	-3.83824600
H	-0.25738100	3.07262400	-3.98838300
C	1.19512700	1.58227200	-3.52465600
H	0.45792400	0.79546700	-3.42033800
C	1.75124500	3.90732100	-3.96111600
H	1.41718300	4.90874100	-4.21829100
C	3.08022000	3.65176000	-3.75210200
H	3.81824900	4.44601700	-3.83571800
C	0.43564700	-2.66866800	6.26652500
H	1.40736400	-2.97949100	6.64014600

C	-0.47713700	-2.01663600	7.14306100
H	-0.20649300	-1.85764600	8.18342300
C	-1.68006300	-1.57318000	6.66453900
H	-2.37949400	-1.05251100	7.31473600
C	0.11336100	-2.89252300	4.95254800
H	0.84070200	-3.35306500	4.29544000
N	1.62254800	-0.39158900	1.49527000
S	2.80153400	-1.17094200	2.33755200
C	4.34908200	-1.11841800	1.24439500
O	2.52686400	-2.60041400	2.50824700
O	3.12983400	-0.32793200	3.48749400
F	4.46907000	-2.25765000	0.56498000
F	4.29955300	-0.09329600	0.39434400
F	5.40838900	-0.97638100	2.04461500
C	2.28227700	3.97743300	1.25640400
C	2.99711300	4.13355900	2.45985000
C	2.93652600	3.33718500	0.19857100
C	4.30088400	3.66754700	2.60307000
H	2.53049800	4.62861800	3.30808100
C	4.25038600	2.87716600	0.33377900
H	2.43881400	3.18683500	-0.75302000
C	4.93777500	3.03641800	1.53299400
H	4.81768400	3.79730800	3.55015700
H	4.72502800	2.38203700	-0.50596100
H	5.95402500	2.66713000	1.63792200
C	1.05408600	6.14262600	1.29460800
H	1.71342900	6.31300900	2.15200900
H	1.62773200	6.45585000	0.41338800
C	-0.17055300	7.03563700	1.44018100
C	-0.71744900	7.60720100	0.35344200
H	-0.25524800	7.38625600	-0.60978800
C	0.12914300	0.65293600	4.02652800
H	-0.60263800	-0.03367900	3.60247900
H	0.97379200	0.06866800	4.38938900
H	-0.33624000	1.15695000	4.88279800
C	-1.90794300	8.51727900	0.25877000
H	-1.63556900	9.46528000	-0.22469500
H	-2.68337900	8.05601100	-0.36693200
H	-2.35781700	8.75118300	1.22686200
C	-0.63478600	7.30969100	2.85454200
H	-1.45205800	8.03267800	2.89650300
H	-0.97698100	6.40339700	3.36845100
H	0.19373300	7.71223800	3.45409300
H	1.57650900	2.15023300	3.26135800

C	-1.75800900	2.11377800	2.35867800
H	-2.34955600	2.75761200	1.70603600
H	-1.84539200	1.07326400	2.03346200
H	-2.20519700	2.15554800	3.36513100

TS-1-1-6SR

1 imaginary frequency

H = -5393.915999

G = -5394.117889

E(M06-2X-DCM) = -5394.845826

C	3.28494900	2.96923400	1.22891800
C	2.74141900	2.63844900	2.66496100
H	3.52588500	2.06172500	3.16389800
H	2.63373500	3.59574500	3.19011700
C	1.42783800	1.93431900	2.88266700
C	2.21641100	3.71014700	0.37719400
H	2.65702500	3.98361100	-0.58742000
H	1.94742700	4.64811400	0.86713800
N	0.98387800	2.97416300	0.14008000
C	-0.19980700	3.60423800	-0.15526200
N	-1.16256800	2.71042400	-0.55410900
C	-2.47173900	2.88988600	-1.02393300
C	-3.31631600	3.95668000	-0.68082900
C	-2.96721000	1.87066500	-1.85423700
C	-4.61775900	3.99191900	-1.18197300
C	-4.26877600	1.92586400	-2.34459600
H	-2.32624900	1.03406400	-2.11385600
C	-5.10844600	2.99119800	-2.02111600
H	-6.11747900	3.04117200	-2.41182500
C	-4.78963900	0.77725500	-3.16192000
C	-5.55121800	5.08414400	-0.72910300
F	-3.83776200	0.25151100	-3.96906400
F	-5.83305200	1.12857500	-3.93843600
F	-5.21917700	-0.24303500	-2.36662200
F	-4.89858800	6.21260800	-0.39281500
F	-6.26178700	4.69816800	0.36420600
F	-6.45519700	5.40010600	-1.68278500
S	-0.41477100	5.27058100	-0.01073100
H	-2.95404200	4.74478800	-0.03695000
C	1.36818200	0.57394700	3.22440500
H	-0.84465100	1.73802500	-0.61020600
H	1.06888300	2.01082900	-0.18076600
H	1.19831600	-0.19159200	2.16158200
O	-1.52858200	-1.47916300	0.19028600

O	0.61706800	-2.25044900	-1.09213700
P	0.05266100	-1.15902800	-0.02559300
O	0.13899900	0.25445500	-0.49978400
C	-3.06522600	-5.28292100	1.09837700
C	-2.55099400	-5.01164200	-0.16300200
C	-2.13767700	-3.71433300	-0.50616400
C	-2.68674500	-2.95001700	1.74719600
C	-3.17674900	-4.24174300	2.01425700
C	0.17443200	-2.12903800	-2.42703500
C	-1.06207700	-2.67055900	-2.76814500
C	-1.59633500	-2.41317300	-4.04160300
C	-0.86104300	-1.71246000	-4.98994000
C	0.42111200	-1.27787700	-4.66222000
C	0.96712200	-1.45817400	-3.37873200
H	-3.63926500	-4.42187700	2.97924800
H	1.02354400	-0.76387300	-5.40503600
C	-1.96562100	-3.64129600	-2.02130100
C	-1.56039100	-5.12084800	-2.32924600
H	-1.73632200	-5.39167600	-3.37482200
H	-0.49018900	-5.24153500	-2.12551700
H	-3.69004800	-2.27094500	-4.61067700
H	-2.99572900	-3.88148500	-4.80040600
C	-2.09972200	-2.73052700	0.48266300
H	-3.40528700	-6.28161100	1.35987900
H	-1.27019300	-1.51504000	-5.97726600
C	-2.38174200	-5.96012000	-1.32908600
H	-3.35316300	-6.25317200	-1.75067800
H	-1.87317400	-6.88655700	-1.03879600
C	-2.99003000	-2.98476800	-4.16534800
C	-3.34148600	-3.32059200	-2.70192600
H	-4.05525600	-4.14342600	-2.60199000
H	-3.78116200	-2.43864300	-2.22426000
C	2.36781100	-0.97976200	-3.15361300
C	3.42053700	-1.92194400	-3.04129500
C	2.65849100	0.40446600	-3.23198400
C	3.20062500	-3.33628300	-3.02771000
C	4.78867100	-1.45925000	-2.97809000
C	4.03446000	0.84823200	-3.22009700
C	4.24197500	-4.22037800	-2.91919800
H	2.18643400	-3.71054600	-3.10446000
C	5.84565800	-2.41416300	-2.85404500
C	5.05849900	-0.09183200	-3.07910200
C	5.58444400	-3.75703200	-2.82116500
H	4.04321000	-5.28854300	-2.90757000

H	6.86690000	-2.04536000	-2.79520600
H	6.09255100	0.24677300	-3.06425500
H	6.39635000	-4.47328600	-2.73006800
C	-2.89856200	-1.90243900	2.79427600
C	-3.71509600	-0.77404200	2.51659000
C	-2.41251500	-2.11811400	4.11154100
C	-4.31861000	-0.53698000	1.23995700
C	-4.00924600	0.17317200	3.57018900
C	-2.77081800	-1.19563500	5.16635700
C	-5.09103800	0.57012800	1.00585800
H	-4.17171200	-1.25606500	0.44340200
C	-4.79798200	1.33073600	3.27641100
C	-3.54320600	-0.07127000	4.86463200
C	-5.31754400	1.53535900	2.02734000
H	-5.53534100	0.70997500	0.02657600
H	-4.98108700	2.04301200	4.07768000
H	-3.79487500	0.62863800	5.65927600
H	-5.89871700	2.42566300	1.80510800
C	1.95295400	2.73621900	-3.46624900
H	1.15989800	3.47467400	-3.54394500
C	1.63981800	1.40746000	-3.33723300
H	0.60191400	1.09853900	-3.30689100
C	3.31254400	3.16279700	-3.49723200
H	3.54195500	4.21742900	-3.62444600
C	4.31985400	2.24319700	-3.36819200
H	5.36185900	2.55480500	-3.38650200
C	-1.11854900	-3.40013700	5.74492200
H	-0.45519900	-4.23040400	5.97075500
C	-1.51388200	-2.51424400	6.78660300
H	-1.16906800	-2.68728100	7.80250000
C	-2.30949000	-1.43862600	6.49848800
H	-2.60515400	-0.74088300	7.27877000
C	-1.54921400	-3.21005600	4.45657600
H	-1.20559200	-3.87696700	3.67572100
N	0.96487100	-1.37977200	1.33018000
S	1.53878200	-2.78698400	1.94429200
C	2.93930100	-3.32212500	0.78337100
O	0.57298000	-3.88589300	1.88199200
O	2.21028300	-2.44904500	3.20241300
F	3.89814500	-3.88412200	1.52871300
F	2.49001100	-4.21910100	-0.09043600
F	3.44932100	-2.27472200	0.13460400
C	0.21300800	0.06974100	4.08864000
H	-0.75928500	0.21509700	3.61361300

H	0.34069400	-0.99561400	4.27977700
H	0.19644000	0.58897400	5.05524700
H	2.33784100	0.14344600	3.48637700
C	0.20023000	2.77916400	3.01604300
H	0.30413000	3.77361800	2.58191400
H	-0.68376000	2.28978700	2.59674500
H	0.00007900	2.89223200	4.09459000
C	4.47283500	3.95659700	1.34715000
C	5.04670700	4.48944900	0.17741200
C	5.03510300	4.35055200	2.57027100
C	6.11491200	5.38249400	0.22951800
H	4.67303800	4.19158300	-0.79693500
C	6.11105200	5.24089000	2.62666600
H	4.65478700	3.96105000	3.50740200
C	6.65462500	5.76705400	1.45754400
H	6.52827000	5.77523700	-0.69578900
H	6.51998700	5.52006200	3.59413500
H	7.48782800	6.46295600	1.50071200
C	3.75153700	1.64384000	0.52530500
H	3.93479300	1.88483400	-0.52834500
H	2.91155200	0.93951700	0.53296000
C	4.98432000	0.93898000	1.08542600
C	4.83359200	-0.12345500	1.89512200
H	3.82019100	-0.44530600	2.12039200
C	6.34004100	1.42964600	0.62146800
H	7.11408200	0.66940000	0.75399900
H	6.30965500	1.68847900	-0.44364600
H	6.66532100	2.32985800	1.15384500
C	5.88790800	-0.98686500	2.52811200
H	5.72591100	-2.03751300	2.25654200
H	6.90728800	-0.71063100	2.24736300
H	5.82082100	-0.93924100	3.62366400

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l imaginary frequency

H = -5393.913932

G = -5394.117082

E(M06-2X-DCM) = -5394.843681

C	3.17183800	2.95992800	1.29391200
C	2.44157100	2.86535900	2.68300900
H	3.15307300	2.44325600	3.39610600
H	2.23102600	3.89484000	2.99430500
C	1.14925900	2.10576300	2.84370200
C	2.22763800	3.65623700	0.27046800

H	2. 76162100	3. 78222900	-0. 67834700
H	1. 97715600	4. 65753100	0. 62567300
N	0. 97483800	2. 95649900	0. 02839100
C	-0. 18404000	3. 59816500	-0. 33607500
N	-1. 14978200	2. 70441900	-0. 72515600
C	-2. 45717700	2. 87543500	-1. 20306900
C	-3. 30055400	3. 95227300	-0. 89081700
C	-2. 95412000	1. 83029800	-1. 99951800
C	-4. 60562900	3. 96752300	-1. 38362700
C	-4. 25817500	1. 86716000	-2. 48469700
H	-2. 31239300	0. 98722100	-2. 23534300
C	-5. 09881000	2. 93949300	-2. 18801600
H	-6. 11069600	2. 97464300	-2. 57293400
C	-4. 77747300	0. 69301900	-3. 26668800
C	-5. 54133000	5. 06769400	-0. 95520200
F	-3. 82946800	0. 15644500	-4. 07122000
F	-5. 83293200	1. 01495000	-4. 03939100
F	-5. 18732600	-0. 31132500	-2. 44139700
F	-4. 89171600	6. 20752000	-0. 65277400
F	-6. 24337300	4. 70721900	0. 15209100
F	-6. 45201400	5. 35419500	-1. 91164400
S	-0. 37353100	5. 27253000	-0. 27444400
H	-2. 93582600	4. 76166900	-0. 27501600
C	1. 13075300	0. 75717000	3. 23179000
H	-0. 84720500	1. 72555800	-0. 73446200
H	1. 04022200	1. 97406500	-0. 23634900
H	1. 02657800	-0. 05419000	2. 19621600
O	-1. 56715700	-1. 50616100	0. 20232200
O	0. 63020000	-2. 28519800	-0. 99010900
P	0. 01065500	-1. 15867000	0. 00842200
O	0. 07608400	0. 23002100	-0. 53742800
C	-3. 06565300	-5. 30951800	1. 17461200
C	-2. 53342600	-5. 05937900	-0. 08384500
C	-2. 12589600	-3. 76585500	-0. 44580200
C	-2. 72577300	-2. 95774700	1. 77837200
C	-3. 20301700	-4. 25048200	2. 06583100
C	0. 22700200	-2. 21442400	-2. 34255000
C	-1. 00254800	-2. 76244300	-2. 70074100
C	-1. 50630100	-2. 53488400	-3. 99220900
C	-0. 74562900	-1. 86303400	-4. 94126500
C	0. 53258100	-1. 43136300	-4. 59591500
C	1. 04717600	-1. 57960300	-3. 29527000
H	-3. 67961600	-4. 41535000	3. 02663900
H	1. 15706900	-0. 94396100	-5. 33841800

C	-1.92376700	-3.71883200	-1.95704600
C	-1.50965100	-5.20289800	-2.23231900
H	-1.66959000	-5.49282300	-3.27531300
H	-0.44203500	-5.31631600	-2.01180500
H	-3.58706200	-2.39175000	-4.60553300
H	-2.89858200	-4.00909600	-4.75410900
C	-2.11932000	-2.75898800	0.51992600
H	-3.40081400	-6.30569800	1.45151800
H	-1.13100100	-1.68814900	-5.94231200
C	-2.34154300	-6.02805400	-1.22936800
H	-3.30556100	-6.33296500	-1.65956600
H	-1.83325100	-6.94686100	-0.91531800
C	-2.90032100	-3.10192300	-4.13414300
C	-3.28402700	-3.41036300	-2.67264000
H	-4.00022200	-4.23120600	-2.57296700
H	-3.73344200	-2.51952800	-2.22087100
C	2.45059000	-1.11306700	-3.06144600
C	3.49040300	-2.06675300	-2.92486100
C	2.75979800	0.26458100	-3.17427000
C	3.25146000	-3.47723300	-2.87402200
C	4.86553000	-1.62208900	-2.88571900
C	4.14147700	0.68999700	-3.17554300
C	4.28159900	-4.37296600	-2.75468300
H	2.23137100	-3.83897800	-2.93053700
C	5.91064100	-2.58861100	-2.75009500
C	5.15318100	-0.26169400	-3.02384400
C	5.63127200	-3.92655100	-2.68222900
H	4.06826900	-5.43760100	-2.71423300
H	6.93776700	-2.23313100	-2.71311600
H	6.19210000	0.06187600	-3.03007000
H	6.43409700	-4.65184100	-2.58270100
C	-2.97518100	-1.89184600	2.79795500
C	-3.79570100	-0.77692500	2.47999700
C	-2.51893800	-2.07880700	4.13016200
C	-4.36004300	-0.56090300	1.18175700
C	-4.13125700	0.18129500	3.51132800
C	-2.92352200	-1.14995800	5.16214600
C	-5.12713900	0.54053100	0.90667800
H	-4.18431200	-1.28967000	0.40015900
C	-4.91596700	1.33058200	3.17630100
C	-3.70480400	-0.04237400	4.82312800
C	-5.39157400	1.51810300	1.90712100
H	-5.53811900	0.66589700	-0.08896000
H	-5.12998100	2.05166100	3.96190600

H	-3.99000800	0.66388300	5.60064200
H	-5.96673000	2.40398500	1.65303700
C	2.08460700	2.59849400	-3.46693500
H	1.30146900	3.34510000	-3.56475100
C	1.75402900	1.27710400	-3.30800500
H	0.71239100	0.98156300	-3.27311300
C	3.44951900	3.00741500	-3.50044800
H	3.69270100	4.05649900	-3.64544800
C	4.44485700	2.07787100	-3.35083800
H	5.49073500	2.37592700	-3.37531600
C	-1.23579600	-3.30725700	5.81218800
H	-0.55663800	-4.11646000	6.06552600
C	-1.68054200	-2.41902800	6.83168900
H	-1.35812500	-2.57087900	7.85824300
C	-2.49348300	-1.36636300	6.50916200
H	-2.82474200	-0.66556900	7.27220100
C	-1.63847600	-3.14468800	4.51114600
H	-1.25838900	-3.81273200	3.74791200
N	0.87640400	-1.27940700	1.40609400
S	1.51637000	-2.62169300	2.09321400
C	3.05560100	-3.01764500	1.06855300
O	0.65841700	-3.80125600	1.96546800
O	2.04642900	-2.21652200	3.39835300
F	3.97485200	-3.53429900	1.88746900
F	2.76230300	-3.90740800	0.12506100
F	3.54486500	-1.90833600	0.50598100
C	-0.04329800	0.23936900	4.06438500
H	-0.99650900	0.31988500	3.53838100
H	0.12309100	-0.80951100	4.30782100
H	-0.12784700	0.79955700	5.00407200
H	2.10207500	0.37687000	3.55549700
C	-0.12040700	2.89524300	2.85927100
H	-0.03368100	3.86526800	2.36880400
H	-0.95812500	2.33916900	2.42801500
H	-0.38409900	3.06648800	3.91641700
C	4.40106100	3.88863400	1.42032100
C	5.17026800	4.16191100	0.27411000
C	4.79977800	4.49620800	2.61900100
C	6.27428000	5.00961000	0.32278100
H	4.91142300	3.70217300	-0.67440800
C	5.91040400	5.34358600	2.67322800
H	4.25413700	4.32208800	3.53949700
C	6.65219000	5.60846400	1.52570700
H	6.84229500	5.20036000	-0.58411400

H	6.18794000	5.79675400	3.62128300
H	7.51312800	6.27004900	1.56586800
C	3.61465000	1.54648500	0.75960200
H	3.72276400	1.63695700	-0.32599500
H	2.78885800	0.84060400	0.91373900
C	4.90257100	0.93129000	1.29766900
C	5.95343500	0.81226000	0.46980200
H	5.82958200	1.18654600	-0.54542800
C	4.91565500	0.42550300	2.72081400
H	5.83164100	-0.12027000	2.95638100
H	4.84239800	1.24326400	3.44993600
H	4.07976900	-0.25972300	2.90758600
C	7.30840900	0.22073900	0.73631500
H	8.09405800	0.97212100	0.57622100
H	7.42756800	-0.16843400	1.75033100
H	7.51361000	-0.60195900	0.03745800

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1 imaginary frequency

H = -5393.907544

G = -5394.113649

E(M06-2X-DCM) = -5394.840969

C	-4.08598800	-0.87157600	1.93790100
C	-3.24015900	-2.04254400	2.59823700
H	-3.52179400	-2.96685600	2.08977700
H	-3.62547800	-2.13737500	3.63003600
C	-1.76642300	-2.08751200	2.86253900
C	-3.65095000	0.54398900	2.37625700
H	-4.42339600	1.25314100	2.07587000
H	-3.60316100	0.60679700	3.47238000
N	-2.40537600	1.00187400	1.78516900
C	-2.09804600	2.32073300	1.64112600
N	-0.94070200	2.50633300	0.91846700
C	-0.41232600	3.68662400	0.36385000
C	-0.42343600	4.92890400	1.01117300
C	0.19716200	3.57654900	-0.89762900
C	0.14648400	6.04030100	0.38635300
C	0.76326400	4.69531500	-1.50167500
H	0.20140500	2.61999700	-1.40985700
C	0.73950300	5.94026900	-0.86927200
H	1.17820800	6.81057100	-1.34366300
C	1.39583200	4.60012000	-2.86200500
C	0.07339200	7.38149800	1.07046100
F	1.29792700	3.35812100	-3.39577000

F	0.82558900	5.45299500	-3.74065700
F	2.71587200	4.91236000	-2.82501700
F	1.08438200	8.19409300	0.68608300
F	-1.07947500	8.02528000	0.78349600
F	0.13683800	7.26381100	2.41433900
S	-3.06681200	3.54928300	2.27162000
H	-0.87866500	5.02620800	1.98588300
C	-1.02604100	-3.21431600	2.44508200
H	-0.48270800	1.64750200	0.60531700
H	-1.63698900	-4.02070400	2.02969200
H	-1.75076200	0.32985300	1.39256500
H	-0.47325800	-2.82229100	1.38518200
O	2.49618400	-1.15613100	0.16156700
O	0.69150700	-0.52974800	-1.61199900
P	0.89257700	-1.11801300	-0.10617000
O	0.10212000	-0.21171700	0.78860000
C	4.72089600	2.38392800	-0.03951700
C	4.40567800	1.68255400	-1.19876600
C	3.71950500	0.45879500	-1.13313100
C	3.65336400	0.64183700	1.30344600
C	4.37494100	1.84198500	1.19858900
C	1.20505500	-1.14156700	-2.77024500
C	2.57375300	-1.10539800	-3.02680600
C	3.08998600	-1.92766500	-4.04116600
C	2.24002500	-2.63719800	-4.88119200
C	0.86191700	-2.49807300	-4.72190800
C	0.30965200	-1.75941000	-3.66346100
H	4.66341800	2.35132300	2.11347600
H	0.18380600	-2.98667400	-5.41515700
C	3.69013800	-0.20250600	-2.50535000
C	3.82216600	1.06236700	-3.42416600
H	4.22025900	0.81611900	-4.41262900
H	2.83124400	1.50297300	-3.56545800
H	4.99280800	-1.34674100	-4.91505800
H	5.04290400	-2.88974200	-4.06930400
C	3.28367900	0.00068400	0.10563700
H	5.24998600	3.33186300	-0.09152400
H	2.63770900	-3.26956900	-5.67072700
C	4.70826800	2.04756100	-2.63428500
H	4.46973100	3.09222000	-2.85695800
H	5.77439300	1.90501700	-2.85975100
C	4.60368300	-1.88613900	-4.04058200
C	4.92289200	-1.13930700	-2.72547400
H	4.97371500	-1.85470100	-1.89710600

H	5.86697000	-0.58605400	-2.75634800
C	-1.17715100	-1.58044600	-3.60829900
C	-2.03009400	-2.68113500	-3.35029100
C	-1.72805400	-0.32067900	-3.96059000
C	-1.53396100	-3.97460000	-2.98608500
C	-3.46324300	-2.51392600	-3.44514700
C	-3.16211400	-0.17645300	-4.07375300
C	-2.38659600	-5.01569500	-2.72338400
H	-0.46458100	-4.12233400	-2.90295700
C	-4.31651500	-3.62798700	-3.16726500
C	-3.98789000	-1.27300700	-3.81272300
C	-3.79747500	-4.84488200	-2.81483800
H	-1.97907100	-5.98034100	-2.43407400
H	-5.39153600	-3.48275100	-3.24586800
H	-5.06594200	-1.15615600	-3.89633600
H	-4.45674300	-5.68369800	-2.60668500
C	3.40544100	0.04776200	2.65586800
C	2.49631700	0.65151200	3.55680900
C	4.17287400	-1.07313800	3.06177800
C	1.70678400	1.79581400	3.21120600
C	2.34114200	0.10696400	4.88836600
C	3.98896900	-1.62253000	4.38630700
C	0.84870000	2.37052300	4.11282800
H	1.79422500	2.20688500	2.21252700
C	1.43594600	0.73805100	5.79932700
C	3.07896300	-1.02028000	5.26028500
C	0.71298100	1.84003900	5.42799100
H	0.25815800	3.23461300	3.82361000
H	1.34263600	0.32389400	6.80087900
H	2.95709500	-1.42779900	6.26216100
H	0.03335100	2.31514400	6.13010300
C	-1.49315000	2.03050000	-4.60316100
H	-0.85589600	2.88709600	-4.80086800
C	-0.92758100	0.83292200	-4.24744200
H	0.15148000	0.75164600	-4.18932800
C	-2.90595100	2.16231700	-4.71640100
H	-3.33673400	3.11659500	-5.00675400
C	-3.71159900	1.08583500	-4.46231500
H	-4.79243500	1.16851700	-4.54986400
C	5.89147200	-2.76230200	2.65050000
H	6.63765200	-3.20175600	1.99409500
C	5.68457600	-3.31675200	3.94534900
H	6.26820000	-4.17646500	4.26283300
C	4.76078100	-2.75831500	4.78628900

H	4. 60196300	-3. 16232800	5. 78341500
C	5. 16329200	-1. 68223900	2. 22534900
H	5. 33990800	-1. 27267200	1. 23765700
N	0. 45885900	-2. 68094900	0. 13992500
S	1. 14754100	-4. 08060800	-0. 33746300
C	2. 81740400	-4. 23930000	0. 53792700
O	0. 33465700	-5. 15565400	0. 23928500
O	1. 51662300	-4. 10376300	-1. 75432700
F	3. 10939400	-5. 54077800	0. 61690700
F	2. 76774200	-3. 73157900	1. 77352000
F	3. 78014100	-3. 62558700	-0. 15243300
C	-1. 11901700	-1. 07158500	3. 74097300
H	-0. 24827400	-0. 63859900	3. 23412200
H	-1. 78381300	-0. 26664900	4. 04501300
H	-0. 73152400	-1. 57206400	4. 63836800
C	0. 14701800	-3. 71146500	3. 29484800
H	-0. 21290100	-4. 01981900	4. 28481400
H	0. 59745600	-4. 57830400	2. 81233800
H	0. 92192600	-2. 95453100	3. 43113300
C	-5. 53108300	-1. 13796900	2. 44040100
C	-6. 15347900	-2. 36617800	2. 15131600
C	-6. 25145500	-0. 22359500	3. 22306700
C	-7. 43268900	-2. 66599800	2. 61524200
H	-5. 64301300	-3. 10747500	1. 54329400
C	-7. 53556600	-0. 52036000	3. 68931000
H	-5. 83190700	0. 74068100	3. 48413400
C	-8. 13415000	-1. 74117700	3. 39009600
H	-7. 88105100	-3. 62427400	2. 36640900
H	-8. 06408300	0. 21534200	4. 28959800
H	-9. 13234800	-1. 97028300	3. 75270000
C	-4. 02426500	-1. 02882300	0. 37521200
H	-4. 29408200	-2. 06256600	0. 13768200
H	-2. 98128800	-0. 91656700	0. 05289300
C	-4. 91387100	-0. 09324200	-0. 43781200
C	-6. 13358700	-0. 51655300	-0. 81153000
H	-6. 43444100	-1. 51866700	-0. 50724000
C	-4. 34550200	1. 25366300	-0. 82391600
H	-4. 36462100	1. 97715800	-0. 00000100
H	-3. 30072200	1. 15552300	-1. 13925400
H	-4. 88945600	1. 70306800	-1. 65717600
C	-7. 18220200	0. 22602700	-1. 59040500
H	-7. 48201000	-0. 33877500	-2. 48439000
H	-8. 09109500	0. 35052600	-0. 98554400
H	-6. 86275600	1. 22083700	-1. 91006900

TS-1-1-6RS-1

1 imaginary frequency

H = -5393.908095

G = -5394.114314

E(M06-2X-DCM) = -5394.840316

C	3.96048100	-1.73155500	-1.62805700
C	2.89743700	-2.84307900	-2.02633300
H	2.93211800	-3.62150400	-1.25965100
H	3.29569900	-3.32642800	-2.93986100
C	1.47422500	-2.69480700	-2.46752600
C	3.74129900	-0.34187200	-2.26755600
H	4.60772900	0.27775500	-2.03269600
H	3.70832200	-0.41917300	-3.36270900
N	2.58091800	0.37355300	-1.76562400
C	2.52255500	1.73252100	-1.68912100
N	1.40665400	2.16229000	-1.00434000
C	1.08245500	3.45455900	-0.54942200
C	1.29079000	4.61918200	-1.29930800
C	0.47451400	3.55132700	0.71333700
C	0.91417100	5.85723600	-0.77472700
C	0.10252600	4.79461500	1.21739800
H	0.31752300	2.65427000	1.30326800
C	0.32264500	5.96082000	0.48158800
H	0.03329900	6.92765000	0.87727600
C	-0.51507000	4.92103600	2.58209100
C	1.19680000	7.10669400	-1.56899200
F	-0.67465100	3.72265400	3.19464200
F	0.23681500	5.68538600	3.40415900
F	-1.73859900	5.50499500	2.52734400
F	0.32492800	8.09676400	-1.26895600
F	2.43581400	7.58563700	-1.32096700
F	1.11685300	6.88567000	-2.89880900
S	3.70751000	2.73696000	-2.34478300
H	1.74705500	4.55815200	-2.27651400
C	0.53183900	-3.63912900	-2.00413400
H	0.79669500	1.42014900	-0.65470300
H	0.97117700	-4.46431000	-1.43540900
H	1.79670900	-0.14139300	-1.37290700
H	-0.01676200	-3.03741200	-1.04970600
O	-2.66580100	-0.71392000	-0.17526100
O	-0.82156600	-0.27212000	1.61084600
P	-1.09472500	-0.96238500	0.16023600
O	-0.11454100	-0.32551200	-0.77800800

C	-4.15866800	3.18965200	-0.37758400
C	-4.02103400	2.55049600	0.85050900
C	-3.58461000	1.21746100	0.92097400
C	-3.40890000	1.16123800	-1.51759100
C	-3.88575000	2.48153500	-1.54845000
C	-1.47173200	-0.67487000	2.79121300
C	-2.81201100	-0.35336400	2.98950400
C	-3.50230000	-0.97241500	4.04399600
C	-2.82736000	-1.76017200	4.96895000
C	-1.44570100	-1.90977900	4.85071600
C	-0.73680000	-1.38464900	3.75935100
H	-4.04018000	2.95159200	-2.51536300
H	-0.89361500	-2.46504300	5.60323500
C	-3.72184600	0.69111800	2.34475200
C	-3.63774100	2.03711800	3.14635400
H	-4.10906800	1.96268700	4.13051000
H	-2.58600200	2.29261900	3.30090000
H	-5.28104600	0.03516200	4.78219000
H	-5.60321600	-1.54217700	4.06974200
C	-3.21074800	0.57338500	-0.25370600
H	-4.49512200	4.22177500	-0.43054100
H	-3.35979300	-2.23550700	5.78869100
C	-4.28967200	3.09703100	2.23424200
H	-3.85767400	4.09215300	2.38050600
H	-5.36938400	3.18408300	2.41971700
C	-4.97949800	-0.64619900	3.97478700
C	-5.11483300	0.02311600	2.58779600
H	-5.27575200	-0.74387300	1.82185000
H	-5.93825900	0.74213400	2.52906100
C	0.75674300	-1.50992600	3.73119500
C	1.37828700	-2.76541100	3.52907400
C	1.54214100	-0.36820000	4.03588700
C	0.63808800	-3.95382000	3.22763800
C	2.81799200	-2.87459900	3.61814300
C	2.97687600	-0.49931800	4.14852900
C	1.26993500	-5.15106000	3.01113400
H	-0.44109700	-3.89602400	3.16069600
C	3.43643900	-4.14521600	3.39275400
C	3.57495900	-1.74353900	3.93150600
C	2.68823100	-5.25246300	3.09436800
H	0.68004600	-6.02970500	2.76628300
H	4.51960100	-4.20988800	3.47093700
H	4.65639700	-1.83239000	4.01142100
H	3.17064400	-6.21203800	2.92663800

C	-3.23345000	0.40597900	-2.79950400
C	-2.18211900	0.72407000	-3.69169500
C	-4.19435700	-0.57510500	-3.15135900
C	-1.19450600	1.72081000	-3.40321900
C	-2.08046200	0.02537900	-4.95474900
C	-4.06675500	-1.28250200	-4.40555900
C	-0.19833300	2.01931500	-4.29658300
H	-1.24252600	2.24311100	-2.45514000
C	-1.02576200	0.36774700	-5.85912300
C	-3.01409400	-0.96593700	-5.26927700
C	-0.11264800	1.33847600	-5.54504200
H	0.54111000	2.77580900	-4.05161000
H	-0.97301900	-0.15827400	-6.80984000
H	-2.93163200	-1.49070900	-6.21928100
H	0.68017700	1.59539000	-6.24221100
C	1.76428200	2.00595400	4.58965000
H	1.30520000	2.97654600	4.75116100
C	0.97850900	0.92777900	4.27266100
H	-0.09602600	1.05285700	4.20844300
C	3.17580000	1.86584800	4.70846600
H	3.78249500	2.72786900	4.97234300
C	3.75964900	0.64639100	4.49399000
H	4.83611200	0.52308600	4.58373600
C	-6.23607700	-1.84104600	-2.69874200
H	-7.08406300	-2.05545500	-2.05399700
C	-6.08851800	-2.55459000	-3.92183900
H	-6.81951100	-3.31010200	-4.19640900
C	-5.03423800	-2.27816900	-4.74921500
H	-4.91620800	-2.80534500	-5.69308000
C	-5.32381700	-0.88812900	-2.32811200
H	-5.45733700	-0.35330000	-1.39500400
N	-0.97593000	-2.59540400	0.09512400
S	-1.96727100	-3.77370800	0.63136100
C	-3.56172700	-3.69001900	-0.38463100
O	-1.35109700	-5.04322000	0.23244300
O	-2.43509900	-3.57524500	2.00473100
F	-4.08851900	-4.91748700	-0.41580500
F	-3.31561200	-3.29305100	-1.63753000
F	-4.44168400	-2.85999000	0.17746200
C	1.07415500	-1.73039200	-3.53176600
H	0.28536800	-1.07052300	-3.14833500
H	1.89119200	-1.11550800	-3.89915900
H	0.63098100	-2.27980700	-4.37141100
C	-0.63491700	-4.06421300	-2.89817800

H	-0.25653600	-4.55777400	-3.80268400
H	-1.25841300	-4.77698100	-2.35840600
H	-1.26234800	-3.22370400	-3.20174200
C	5.31527700	-2.30891500	-2.11650800
C	5.72132600	-3.58345800	-1.67907000
C	6.16580000	-1.63184100	-3.00322800
C	6.92066600	-4.15302500	-2.10103800
H	5.10252600	-4.14293800	-0.98343800
C	7.37087800	-2.20029400	-3.42709000
H	5.91320200	-0.64590900	-3.37475500
C	7.75591800	-3.46190600	-2.98029700
H	7.20376400	-5.13697400	-1.73649200
H	8.00722300	-1.64495200	-4.11090800
H	8.69333100	-3.90126800	-3.30972900
C	3.96532300	-1.59421400	-0.05858700
H	4.07609900	-2.59898200	0.36777300
H	2.97482900	-1.24524200	0.25356400
C	5.03218400	-0.67750400	0.52939000
C	4.71372900	0.58658300	0.85518200
H	3.68320000	0.89975300	0.69767700
C	6.40675400	-1.27115300	0.75555300
H	6.32548500	-2.27932100	1.18209800
H	6.98087300	-1.37135800	-0.17228600
H	7.00146200	-0.66799600	1.44614900
C	5.60318100	1.67209200	1.38860100
H	5.64772100	2.49858600	0.66680900
H	5.19098400	2.08584100	2.31729700
H	6.62768900	1.34360800	1.58306400

TS-1-1-6RS-2

1 imaginary frequency

H = -5393.904901

G = -5394.110646

E(M06-2X-DCM) = -5394.837003

C	-3.79435700	2.02884300	1.70029900
C	-3.53465500	0.98070700	2.86033600
H	-4.33473400	0.24389000	2.81514800
H	-3.66871100	1.53981100	3.80008400
C	-2.24816500	0.24403500	3.09256400
C	-2.65816600	3.06378000	1.53755100
H	-3.00239300	3.82898600	0.83932900
H	-2.48599500	3.58457300	2.48885100
N	-1.38806900	2.57925100	1.01794700
C	-0.38920600	3.44993500	0.69379100

N	0. 73597700	2. 81245100	0. 22667100
C	1. 92943500	3. 34215900	-0. 28786100
C	2. 50971400	4. 54608700	0. 14016300
C	2. 59797700	2. 57097500	-1. 25371300
C	3. 71732600	4. 96967500	-0. 41619500
C	3. 80465700	3. 01060100	-1. 79429500
H	2. 14964300	1. 64556700	-1. 59987500
C	4. 37498100	4. 21728000	-1. 38712800
H	5. 30847100	4. 56126700	-1. 81529200
C	4. 52654400	2. 16395900	-2. 80482600
C	4. 29188500	6. 29535000	0. 01323400
F	3. 67584700	1. 38022500	-3. 51699500
F	5. 21885600	2. 90935000	-3. 69008400
F	5. 42050000	1. 32679000	-2. 21882500
F	5. 63413300	6. 33586600	-0. 15112300
F	3. 77688500	7. 31861200	-0. 70372000
F	4. 03551800	6. 55558400	1. 31370300
S	-0. 57595800	5. 11942400	0. 85965200
H	2. 01470200	5. 14504300	0. 89046400
C	-2. 20846000	-1. 16022500	2. 98788100
H	0. 67042000	1. 79263300	0. 17587100
H	-3. 19067700	-1. 62759800	2. 87761500
H	-1. 21906300	1. 58840200	0. 86965400
H	-1. 78211000	-1. 38483900	1. 81463300
O	1. 33408200	-2. 33963100	0. 45108700
O	0. 30063900	-0. 99417500	-1. 52819900
P	0. 15564200	-1. 28875000	0. 06273300
O	0. 23344100	0. 04601700	0. 73755200
C	5. 33839900	-1. 23991000	-0. 12520400
C	4. 58686900	-1. 74839000	-1. 17830200
C	3. 26444900	-2. 17878600	-0. 97746400
C	3. 43871900	-1. 56413300	1. 38064500
C	4. 77067400	-1. 18380400	1. 14630800
C	0. 24943900	-1. 94847600	-2. 56001000
C	1. 28837100	-2. 86529200	-2. 70982000
C	1. 10893500	-3. 95117000	-3. 58215400
C	0. 00021800	-4. 01194500	-4. 41759800
C	-0. 92160200	-2. 96762200	-4. 39164700
C	-0. 83807200	-1. 92080900	-3. 45677700
H	5. 35904800	-0. 82970700	1. 98763700
H	-1. 74765300	-2. 96120300	-5. 09537700
C	2. 74163300	-2. 85656100	-2. 23802400
C	3. 63362600	-2. 14582200	-3. 31734300
H	3. 70485200	-2. 72318600	-4. 24333300

H	3.18917600	-1.17526200	-3.56222300
H	2.88463600	-4.91897000	-4.37635600
H	1.92041700	-5.95547700	-3.33131500
C	2.68750800	-2.01377800	0.27809100
H	6.35800400	-0.90026900	-0.28475200
H	-0.13186600	-4.83998800	-5.10927700
C	4.99067000	-1.91932300	-2.62411600
H	5.52269000	-1.04578400	-3.01123200
H	5.65647400	-2.78493600	-2.74766700
C	2.26385300	-4.92389800	-3.47003900
C	3.04218100	-4.39077100	-2.24582300
H	2.64088000	-4.83334000	-1.32758100
H	4.11443900	-4.60621500	-2.28503800
C	-1.83688900	-0.80933400	-3.53053400
C	-3.22698400	-1.09422900	-3.46891200
C	-1.39679300	0.51036900	-3.82174400
C	-3.74546300	-2.39625600	-3.16601100
C	-4.18430000	-0.04211700	-3.72851200
C	-2.36976600	1.56392500	-4.00713900
C	-5.09292500	-2.65004600	-3.18803100
H	-3.05792600	-3.18524100	-2.89204900
C	-5.57981900	-0.35284400	-3.74977000
C	-3.73218200	1.25776600	-3.96558800
C	-6.02631100	-1.62265900	-3.50354600
H	-5.45311600	-3.64819800	-2.95360100
H	-6.27918500	0.44942800	-3.97259500
H	-4.45859200	2.04842200	-4.14328800
H	-7.08916300	-1.84760700	-3.53237900
C	2.93211300	-1.54428700	2.78991300
C	2.74454000	-0.31185000	3.46128300
C	2.77899100	-2.76768900	3.48969500
C	2.88027000	0.95541900	2.80624400
C	2.40310600	-0.30727800	4.86700800
C	2.41934800	-2.74842500	4.89023700
C	2.71332200	2.13319600	3.48782200
H	3.11344000	0.97356200	1.74814300
C	2.23981300	0.94441300	5.54129700
C	2.24577400	-1.52236900	5.53949500
C	2.39421300	2.13146600	4.87634100
H	2.82235400	3.07881400	2.96467300
H	1.99684200	0.92940800	6.60148200
H	1.99348800	-1.51443800	6.59821300
H	2.27348300	3.07545200	5.40059900
C	0.36985200	2.14701000	-4.26836600

H	1. 42507100	2. 36997600	-4. 39247900
C	-0. 01866300	0. 86101300	-3. 99489500
H	0. 73505900	0. 08588800	-3. 92724700
C	-0. 59254500	3. 18793200	-4. 39397200
H	-0. 26619300	4. 20398300	-4. 59682100
C	-1. 92364300	2. 89667800	-4. 27413800
H	-2. 67448500	3. 67479100	-4. 38969100
C	2. 85378900	-5. 20866800	3. 58951300
H	3. 02787900	-6. 16342700	3. 10071100
C	2. 47828900	-5. 18387100	4. 96262000
H	2. 36510500	-6. 11733000	5. 50697200
C	2. 27025100	-3. 98625800	5. 59112000
H	1. 99402600	-3. 95163200	6. 64239600
C	2. 99980500	-4. 04506700	2. 88080800
H	3. 29081700	-4. 08559300	1. 83750600
N	-1. 20365300	-2. 06955700	0. 55566400
S	-1. 76809400	-3. 57379400	0. 27999300
C	-0. 56051900	-4. 80815100	1. 04337300
O	-2. 98229700	-3. 70596800	1. 09018700
O	-1. 76420700	-3. 94713000	-1. 13502000
F	-1. 21334500	-5. 96119600	1. 21013200
F	-0. 11356500	-4. 38670100	2. 23029000
F	0. 48070300	-5. 01612100	0. 23333000
C	-1. 06831300	0. 98082500	3. 62845900
H	-0. 16462200	0. 73146700	3. 06133900
H	-1. 20287600	2. 06142500	3. 63927400
H	-0. 88253100	0. 63649600	4. 65662600
C	-1. 22890600	-1. 96099900	3. 84763700
H	-1. 41837800	-1. 77757300	4. 91272600
H	-1. 36323300	-3. 02496000	3. 65777900
H	-0. 18673400	-1. 70972300	3. 64009500
C	-5. 07319100	2. 80516700	2. 13334700
C	-6. 20864500	2. 10724200	2. 58774700
C	-5. 16323300	4. 20742000	2. 10828900
C	-7. 36610800	2. 76807500	2. 99475000
H	-6. 20944700	1. 02451700	2. 62284000
C	-6. 32411400	4. 87350800	2. 51209800
H	-4. 33190900	4. 82001600	1. 78284200
C	-7. 43299900	4. 16082100	2. 95812300
H	-8. 21791700	2. 18701300	3. 33845600
H	-6. 34768300	5. 95942000	2. 47836500
H	-8. 33393600	4. 67951500	3. 27413400
C	-4. 00803800	1. 31102300	0. 31156900
H	-3. 14096100	0. 66352900	0. 12420800

H	-3.96165800	2.10484700	-0.44196200
C	-5.27967100	0.50854000	0.08270700
C	-6.32396600	1.10880900	-0.51143000
H	-6.20519700	2.15489000	-0.79666000
C	-5.29459300	-0.94230400	0.51466800
H	-4.30390200	-1.39926700	0.43287600
H	-5.62036700	-1.07120000	1.55853400
H	-5.97052500	-1.54345800	-0.09863500
C	-7.68326400	0.53848700	-0.79392700
H	-8.44132500	1.04052300	-0.17552500
H	-7.97141900	0.70590700	-1.83957000
H	-7.74964600	-0.53393200	-0.59378800

TS-1-1-6RR

l imaginary frequency

H = -5393.903756

G = -5394.108715

E(M06-2X-DCM) = -5394.834826

C	-2.77951300	3.92113000	1.25384600
C	-2.64164800	3.20757400	2.64601300
H	-3.63905200	2.87747100	2.94148200
H	-2.34707200	4.00128500	3.34839200
C	-1.65684800	2.10360300	2.92355100
C	-1.43190600	4.51039000	0.77058600
H	-1.61697900	5.26665100	-0.00273300
H	-0.95499900	5.05511100	1.59110600
N	-0.49734300	3.51440200	0.27398200
C	0.79622400	3.81585000	-0.05214600
N	1.47524000	2.71459900	-0.51189700
C	2.73733000	2.55615600	-1.09955000
C	3.70591700	3.55725200	-1.25997200
C	3.01954900	1.25766300	-1.57292800
C	4.92202000	3.25017900	-1.87899100
C	4.23156700	0.97981500	-2.19004800
H	2.27186200	0.47974800	-1.47093700
C	5.20297200	1.97258800	-2.35066300
H	6.14433300	1.75644100	-2.84186600
C	4.51242200	-0.39582200	-2.72710000
C	5.96949600	4.33010600	-1.97708600
F	3.44182700	-1.21969100	-2.62314000
F	4.85024000	-0.35486900	-4.03909500
F	5.53893200	-1.00096100	-2.08483600
F	6.87185800	4.07074400	-2.95019600
F	5.42668800	5.53722200	-2.23781300

F	6.66225800	4.45167400	-0.82006700
S	1.41074500	5.37188400	0.15537000
C	-3.69506600	5.19087800	1.49056600
H	-3.85359600	5.63966900	0.50478400
H	-3.10340600	5.91508100	2.06800500
H	3.50511000	4.56081000	-0.91325000
C	-2.08917100	0.78945900	3.16890600
H	1.00844500	1.81987600	-0.33383800
H	-3.17201500	0.67659400	3.25755600
H	-0.88930900	2.64454400	-0.07173400
H	-1.92230900	0.15318100	2.05999500
O	0.44113000	-2.22891500	1.23696300
O	-0.20728400	-1.46307100	-1.19215600
P	-0.27797000	-1.03976200	0.37824900
O	0.38489900	0.29235800	0.49226500
C	4.54893400	-2.84273300	0.63814500
C	3.61200700	-3.41354800	-0.21490100
C	2.23769300	-3.26856200	0.02957200
C	2.73451200	-1.95550900	2.02315200
C	4.10215300	-2.15641300	1.76464600
C	-0.58579900	-2.66746800	-1.81122600
C	0.05201800	-3.86306700	-1.47132600
C	-0.51861100	-5.07892400	-1.88201200
C	-1.57660100	-5.09385600	-2.78148600
C	-2.02721700	-3.88369400	-3.30073500
C	-1.56230600	-2.63941400	-2.83272400
H	4.82047300	-1.75324000	2.47214400
H	-2.77251500	-3.88550200	-4.08870700
C	1.44194900	-4.16135400	-0.90819200
C	2.45428900	-4.28516100	-2.10459400
H	2.28180400	-5.18724300	-2.69805900
H	2.32717400	-3.42421300	-2.76738300
H	0.74869700	-6.83572000	-2.03797700
H	-0.46544000	-6.94929600	-0.77021100
C	1.81540300	-2.47457400	1.09092100
H	5.61322400	-2.94558100	0.44525800
H	-2.00877900	-6.03106600	-3.12263900
C	3.85350300	-4.23328000	-1.45972800
H	4.60277600	-3.77487900	-2.11369700
H	4.22041900	-5.23746400	-1.20542200
C	0.21700500	-6.25400900	-1.27290900
C	1.19698500	-5.57509600	-0.28997900
H	0.72163500	-5.45517400	0.68974100
H	2.12756500	-6.13371000	-0.14861900

C	-2.03655200	-1.41752200	-3.55977200
C	-3.42933000	-1.21878800	-3.77092600
C	-1.09808300	-0.58805100	-4.23711300
C	-4.43886200	-1.98188200	-3.09655300
C	-3.87898600	-0.22113000	-4.71582000
C	-1.57380900	0.46149600	-5.11298400
C	-5.76983800	-1.82791800	-3.39104100
H	-4.14034800	-2.67173100	-2.31914400
C	-5.27544600	-0.10201300	-5.00539000
C	-2.94370600	0.60435400	-5.34165300
C	-6.19851400	-0.89321700	-4.37591200
H	-6.50825300	-2.42141900	-2.85865000
H	-5.58491500	0.63571800	-5.74241000
H	-3.28769300	1.36196500	-6.04335800
H	-7.25586600	-0.79861300	-4.60892500
C	2.37108700	-1.30022200	3.31923100
C	2.72973800	0.04970800	3.55438500
C	1.82898900	-2.08640800	4.36855300
C	3.24795600	0.90219800	2.52543700
C	2.56962400	0.61383700	4.87660700
C	1.65671200	-1.50279300	5.68065800
C	3.59859700	2.20221600	2.78476200
H	3.34460400	0.50747700	1.52091600
C	2.95772300	1.97206100	5.10687100
C	2.04077300	-0.17643800	5.90065700
C	3.46052500	2.74513000	4.09466200
H	3.97685400	2.83032500	1.98352400
H	2.84463400	2.37602600	6.11050900
H	1.92869800	0.24944600	6.89601200
H	3.75062400	3.77536600	4.28091500
C	1.19235000	0.05017900	-4.83464400
H	2.26093300	-0.12234100	-4.75648000
C	0.32177100	-0.76503800	-4.15800000
H	0.72293700	-1.57106100	-3.55818500
C	0.71289000	1.11328600	-5.64918800
H	1.41780300	1.75576000	-6.16949400
C	-0.63406900	1.30475300	-5.78505600
H	-1.02187100	2.09627900	-6.42213300
C	0.94026500	-4.19049800	5.24027500
H	0.66689200	-5.23038400	5.08341600
C	0.75708000	-3.60504400	6.52486700
H	0.34301900	-4.20002100	7.33421900
C	1.11067700	-2.29990900	6.73519800
H	0.98626100	-1.84186300	7.71369500

C	1.46090700	-3.46053400	4.20377300
H	1.60150500	-3.92946200	3.23702700
N	-1.77801900	-0.97752800	1.06277300
S	-3.00472400	-2.04120200	1.11975400
C	-2.41831200	-3.53526900	2.10789200
O	-4.04922300	-1.43343600	1.95036500
O	-3.33479400	-2.61788500	-0.18309800
F	-3.49152200	-4.25425500	2.44585500
F	-1.77094400	-3.17323600	3.22032600
F	-1.60618900	-4.29292400	1.36270500
C	-3.43479500	3.03176900	0.18638100
C	-4.15026600	1.86738200	0.49550800
C	-3.42150100	3.44777800	-1.15865000
C	-4.83841300	1.15363800	-0.48726900
H	-4.19976400	1.49397000	1.50945900
C	-4.11291000	2.74180300	-2.14032300
H	-2.87712100	4.34170700	-1.44879300
C	-4.83347900	1.59359700	-1.80759800
H	-5.36920600	0.24825200	-0.20955500
H	-4.08151000	3.08652900	-3.17015100
H	-5.37321400	1.04441300	-2.57018100
C	-5.04084000	4.99059000	2.17655800
C	-6.10067200	4.57754100	1.46140400
H	-5.94239900	4.39309200	0.39927000
C	-5.09753400	5.36083700	3.64250100
H	-6.08644200	5.21050400	4.08087500
H	-4.38213800	4.78547300	4.24415200
H	-4.83311100	6.41885800	3.77884800
C	-0.22314900	2.45575700	3.13057000
H	0.42672000	1.78591600	2.55718800
H	0.01283600	3.48813200	2.87798200
H	0.02994100	2.28647100	4.18770500
C	-1.29326300	-0.10639500	4.12021300
H	-1.24800800	0.34094200	5.12054800
H	-1.78177200	-1.07632400	4.20213000
H	-0.27190100	-0.27407100	3.77607100
C	-7.50760400	4.32519700	1.92346400
H	-8.21328200	4.97460600	1.38746000
H	-7.80399600	3.29234100	1.69666400
H	-7.65352800	4.48661900	2.99455700

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l imaginary frequency

H = -5393.905723

G = -5394.111676

E(M06-2X-DCM) = -5394.834766

C	-3.25493400	3.76364100	0.38443800
C	-3.22161300	3.18890100	1.84460500
H	-4.20065900	2.75213600	2.04784600
H	-3.14571100	4.07129700	2.49992300
C	-2.15249500	2.27769400	2.38279500
C	-1.90808300	4.40099700	-0.04096700
H	-2.07150800	5.04254300	-0.91613200
H	-1.55117800	5.07433000	0.74400000
N	-0.86233700	3.43402100	-0.32933100
C	0.42967700	3.80558700	-0.58229800
N	1.23183200	2.72051100	-0.83845800
C	2.54960500	2.60692900	-1.30165600
C	3.41668500	3.67007700	-1.59236700
C	3.00404300	1.28722300	-1.50522200
C	4.70349700	3.40293300	-2.07024400
C	4.28390100	1.04837900	-1.98761300
H	2.33696600	0.45748800	-1.30279300
C	5.15464000	2.10359400	-2.27532300
H	6.14911700	1.91547100	-2.66227400
C	4.75228300	-0.35871300	-2.23357100
C	5.63509500	4.56339900	-2.31212800
F	3.75942100	-1.26774500	-2.08003000
F	5.22998900	-0.50755000	-3.49346700
F	5.75283500	-0.72416700	-1.39835900
F	6.62411100	4.24373400	-3.17728900
F	4.98696700	5.63469000	-2.81448900
F	6.23084100	4.96583800	-1.16496400
S	0.90246500	5.42237900	-0.51895000
C	-4.25380000	4.99021300	0.43324400
H	-4.36087700	5.35442700	-0.59578400
H	-3.74643900	5.78576500	0.99383800
H	3.08564600	4.68892700	-1.45229700
C	-2.46777200	0.97636000	2.80790900
H	0.83317200	1.81959900	-0.55629100
H	-3.53654600	0.74832400	2.81435000
H	-1.15725300	2.50447800	-0.60983100
H	-2.11765000	0.20104400	1.83432500
O	0.51908800	-1.99998400	1.59775400
O	0.05774100	-1.67137400	-0.96797200
P	-0.21040500	-1.03151300	0.50421900
O	0.31190900	0.36542600	0.46648700
C	4.70401600	-2.26790400	1.45942400

C	3.91241800	-3.05598200	0.63254400
C	2.51309700	-3.01796600	0.73125500
C	2.68784100	-1.37063300	2.52103700
C	4.08693300	-1.46634900	2.41680800
C	-0.14950200	-2.98674700	-1.42016400
C	0.55105600	-4.04767200	-0.84111900
C	0.13102500	-5.36221300	-1.10223100
C	-0.82633400	-5.61720400	-2.07554800
C	-1.32486300	-4.54959300	-2.81664300
C	-1.01709800	-3.20932200	-2.51338200
H	4.69162600	-0.88676500	3.10784900
H	-1.98516100	-4.74355500	-3.65503200
C	1.89706500	-4.11726900	-0.11850900
C	3.03297900	-4.31579900	-1.18710600
H	3.00106300	-5.30980400	-1.64163900
H	2.89944600	-3.58197500	-1.98722800
H	1.55432600	-6.98577700	-0.86784100
H	0.23201600	-7.03122100	0.29135000
C	1.91775700	-2.11994100	1.61095300
H	5.78725000	-2.28837700	1.37765800
H	-1.14043500	-6.63340300	-2.29963100
C	4.34960300	-4.02491000	-0.43983000
H	5.11839200	-3.59608600	-1.09129900
H	4.77527200	-4.93660000	0.00212600
C	0.89944500	-6.35327400	-0.25342700
C	1.71246300	-5.44026500	0.69164600
H	1.13137700	-5.22397100	1.59485000
H	2.66828800	-5.87528800	1.00020100
C	-1.51832900	-2.16239800	-3.46190500
C	-2.89571200	-2.13112700	-3.81579500
C	-0.58970800	-1.35844400	-4.18236900
C	-3.90051000	-2.87559900	-3.11390500
C	-3.33197700	-1.33433100	-4.94049700
C	-1.06279200	-0.50328900	-5.24993000
C	-5.20644800	-2.88968800	-3.53385100
H	-3.62221200	-3.41302100	-2.21780300
C	-4.69947300	-1.39242900	-5.35851800
C	-2.41140700	-0.52744800	-5.61002700
C	-5.61307800	-2.15882100	-4.68627400
H	-5.94231700	-3.46230700	-2.97568400
H	-4.99460000	-0.80868800	-6.22771700
H	-2.74727700	0.08150900	-6.44719700
H	-6.64790600	-2.19947400	-5.01598200
C	2.13777700	-0.56391700	3.65604400

C	2.34248700	0.83707400	3.69337000
C	1.56946500	-1.23094500	4.77177700
C	2.87760500	1.56985700	2.58403300
C	1.99897000	1.57981300	4.88608200
C	1.21433700	-0.47227600	5.95082200
C	3.07387800	2.92521800	2.65190900
H	3.11208400	1.03586700	1.67080700
C	2.23077200	2.99178100	4.91922400
C	1.44860900	0.90592800	5.97967400
C	2.75454300	3.64782900	3.83750900
H	3.46702100	3.45879600	1.79154100
H	1.98029500	3.53275000	5.82910200
H	1.19867400	1.46712100	6.87815800
H	2.92373900	4.72034900	3.87285400
C	1.68753200	-0.60062800	-4.68156100
H	2.75392300	-0.65517100	-4.48808200
C	0.82528600	-1.38380700	-3.95800700
H	1.23093100	-2.04657400	-3.20526900
C	1.20392500	0.27579400	-5.69219600
H	1.90099900	0.89671900	-6.24801500
C	-0.13475800	0.31485500	-5.96756200
H	-0.52276000	0.96050100	-6.75198600
C	0.79690300	-3.25704000	5.90092500
H	0.63778200	-4.33192200	5.89527600
C	0.43398600	-2.50209300	7.05196600
H	-0.00142500	-3.00499600	7.91104300
C	0.64280100	-1.14981100	7.07326500
H	0.38002800	-0.56128200	7.94924200
C	1.34826000	-2.64546500	4.80536200
H	1.62719600	-3.24098700	3.94405800
N	-1.77357500	-1.02889300	1.03674700
S	-2.89684300	-2.19682600	1.15017300
C	-2.29545900	-3.45110100	2.42244100
O	-4.07859900	-1.58024600	1.76149000
O	-3.02599100	-2.99793800	-0.06659900
F	-3.33336500	-4.21520200	2.77078800
F	-1.80811400	-2.85590000	3.51581100
F	-1.34388000	-4.22685300	1.89250500
C	-3.72921200	2.73627300	-0.65696100
C	-4.16679600	1.44665200	-0.32606900
C	-3.79539600	3.11809600	-2.01034400
C	-4.68425500	0.58391900	-1.29540400
H	-4.13373100	1.08767200	0.69384200
C	-4.31278500	2.26139900	-2.97821700

H	-3.45118800	4.10179700	-2.31703000
C	-4.77319000	0.99222300	-2.62328500
H	-5.01196100	-0.40844000	-1.00148700
H	-4.35631600	2.58837500	-4.01374200
H	-5.18269400	0.32544900	-3.37343200
C	-5.63527200	4.78631700	1.03123100
C	-5.90389300	5.30528200	2.24282200
H	-5.09738900	5.84352500	2.74498300
C	-6.65248600	4.06731300	0.17513100
H	-7.66104800	4.12163600	0.59093000
H	-6.68096900	4.50558600	-0.83083500
H	-6.40093000	3.00978000	0.03997300
C	-0.79499700	2.82852900	2.66168100
H	-0.02146800	2.17161700	2.24888500
H	-0.64539000	3.83820900	2.28417700
H	-0.63495200	2.83310300	3.74965500
C	-1.69005300	0.34099900	3.96127000
H	-1.80050900	0.93923700	4.87392300
H	-2.07908600	-0.65671300	4.15950200
H	-0.62540500	0.24785200	3.74294300
C	-7.18781200	5.26321700	3.02244200
H	-7.03525200	4.77392600	3.99426900
H	-7.54329800	6.27961500	3.23990100
H	-7.99067400	4.72999400	2.50786000

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l imaginary frequency

H = -5393.904660

G = -5394.111344

E(M06-2X-DCM) = -5394.834900

C	-1.93979600	3.49160400	2.91063400
C	-1.46645700	2.51742600	4.06115400
H	-2.35354300	2.23237100	4.63074100
H	-0.84468300	3.13073500	4.72716500
C	-0.66125100	1.27590200	3.79521300
C	-0.73592700	4.11491600	2.17503900
H	-1.07929800	4.96763000	1.58035500
H	-0.04565500	4.53460900	2.91448700
N	0.00954900	3.19137000	1.33051400
C	1.16365100	3.55408400	0.69381600
N	1.63872700	2.55005800	-0.11291200
C	2.68939900	2.49526800	-1.03708100
C	3.74791100	3.40863000	-1.13809700
C	2.65363300	1.39629100	-1.92002000

C	4. 73788500	3. 21385900	-2. 10721100
C	3. 64490000	1. 22740800	-2. 87678800
H	1. 83081700	0. 69307100	-1. 86041400
C	4. 70354100	2. 13485500	-2. 98403400
H	5. 47181000	2. 00741400	-3. 73747300
C	3. 57737200	0. 07915000	-3. 84438000
C	5. 89906600	4. 17458900	-2. 14544300
F	2. 46721500	-0. 67857000	-3. 67019000
F	3. 55844200	0. 51243800	-5. 12766600
F	4. 64182300	-0. 75042900	-3. 73328500
F	6. 54989700	4. 13506400	-3. 32969300
F	5. 50619400	5. 44834300	-1. 93967300
F	6. 80923100	3. 88420900	-1. 18520400
S	1. 86518500	5. 06844600	0. 93402800
C	-2. 63788500	4. 67255900	3. 70408000
H	-1. 86866400	5. 11504500	4. 35038800
H	-3. 38067000	4. 21391000	4. 36945100
H	3. 78390900	4. 26433400	-0. 47869300
C	-1. 25693600	0. 00371500	3. 80222900
H	1. 13467900	1. 66186800	-0. 03710400
H	-2. 30311700	-0. 00582900	4. 11369800
H	-0. 45644600	2. 34320300	1. 02320100
H	-1. 42085800	-0. 34891600	2. 56813900
O	0. 41245100	-2. 54364000	0. 61605600
O	-0. 76153500	-1. 17915900	-1. 29822200
P	-0. 38525600	-1. 15635600	0. 28563700
O	0. 41512200	0. 08181400	0. 52187600
C	4. 16357800	-3. 11195200	-1. 18034600
C	2. 99269800	-3. 41165900	-1. 86627000
C	1. 74368400	-3. 29358100	-1. 23713600
C	2. 84594700	-2. 56091500	0. 81019400
C	4. 07987000	-2. 73179300	0. 15665300
C	-1. 39064900	-2. 18169200	-2. 05826900
C	-0. 79510600	-3. 43790500	-2. 19626500
C	-1. 55508500	-4. 49848100	-2. 71681000
C	-2. 80235200	-4. 26378800	-3. 27987700
C	-3. 26201000	-2. 95248900	-3. 35645900
C	-2. 58816300	-1. 87743600	-2. 74545800
H	4. 98764200	-2. 55291600	0. 72486500
H	-4. 17869700	-2. 73894900	-3. 89532600
C	0. 65968400	-3. 89938800	-2. 11269300
C	1. 32113100	-3. 74028400	-3. 52971300
H	0. 92129300	-4. 45566300	-4. 25358600
H	1. 11169400	-2. 73536400	-3. 90802900

H	-0.52728600	-6.18612900	-3.61782300
H	-1.38759600	-6.58961500	-2.13748000
C	1.67707100	-2.78731200	0.05710400
H	5.13133400	-3.19496800	-1.66731000
H	-3.38601600	-5.07502600	-3.70734100
C	2.83597800	-3.89231200	-3.28911800
H	3.43623500	-3.30263200	-3.98962200
H	3.15949600	-4.93775800	-3.38937800
C	-0.79571900	-5.80505600	-2.62327900
C	0.45565300	-5.41752500	-1.80466800
H	0.25441100	-5.53668500	-0.73432400
H	1.33923000	-6.01429900	-2.05171400
C	-3.12567600	-0.50318200	-3.00521900
C	-4.50382200	-0.23040200	-2.77931600
C	-2.32136800	0.45334000	-3.68713000
C	-5.37310100	-1.12606700	-2.07356100
C	-5.08747500	0.99197400	-3.28543100
C	-2.91024900	1.70181900	-4.12251600
C	-6.71396300	-0.86845600	-1.94172900
H	-4.95135300	-2.00592700	-1.60829100
C	-6.49118500	1.22168700	-3.12928300
C	-4.27420700	1.92928100	-3.92627900
C	-7.29030600	0.31152200	-2.49124700
H	-7.34223000	-1.56793700	-1.39687900
H	-6.90845100	2.14045300	-3.53508700
H	-4.71729700	2.85049700	-4.30017300
H	-8.35652200	0.49359200	-2.38552000
C	2.88514500	-2.25695100	2.27534700
C	3.46138200	-1.04455600	2.72870900
C	2.51449800	-3.26091000	3.20743900
C	3.82856200	0.01748400	1.83900600
C	3.69497500	-0.84598700	4.14220000
C	2.73158200	-3.03743700	4.61999500
C	4.40299400	1.17250800	2.30378700
H	3.63081300	-0.09736600	0.77977500
C	4.30424000	0.37116300	4.58447700
C	3.32285300	-1.84437100	5.04633400
C	4.65347100	1.35149500	3.69463700
H	4.66414700	1.96357600	1.60688100
H	4.48604600	0.49761200	5.64945400
H	3.50500500	-1.69344800	6.10872700
H	5.11623000	2.27087700	4.04234900
C	-0.20979900	1.17678500	-4.70166200
H	0.82484500	0.96819000	-4.95490800

C	-0.94875000	0.23305600	-4.03586900
H	-0.48164500	-0.70865200	-3.78008500
C	-0.78598700	2.42225900	-5.07703900
H	-0.18273600	3.16237900	-5.59535500
C	-2.10164000	2.66921700	-4.79848700
H	-2.56730600	3.60519400	-5.09823400
C	1.61056700	-5.46794500	3.74557800
H	1.18533300	-6.41287200	3.41858000
C	1.80645100	-5.23271400	5.13572100
H	1.52560300	-5.99578000	5.85636000
C	2.35560200	-4.05175600	5.55560000
H	2.52283900	-3.86225600	6.61334900
C	1.95556400	-4.52042900	2.81752600
H	1.80704500	-4.72561600	1.76406200
N	-1.64344100	-1.21152800	1.34940200
S	-2.92274300	-2.20786400	1.48318900
C	-2.26034000	-3.93192100	1.85786100
O	-3.63852200	-1.81663900	2.69979900
O	-3.63823000	-2.39784900	0.22223300
F	-3.28176500	-4.68387100	2.27612100
F	-1.32182000	-3.90774100	2.80950500
F	-1.74214500	-4.48232300	0.75383800
C	-2.95190900	2.82128400	1.97443000
C	-3.93078300	1.94537300	2.47193800
C	-3.00567900	3.14719000	0.60947500
C	-4.91876500	1.41358000	1.64587200
H	-3.94591700	1.67204500	3.52190600
C	-3.99860900	2.62261500	-0.21826500
H	-2.28180500	3.83003100	0.17858800
C	-4.96079900	1.75409500	0.29439300
H	-5.64731300	0.72348800	2.06076500
H	-4.01105500	2.88808900	-1.27046600
H	-5.72695300	1.34158400	-0.35205000
C	-3.31207700	5.78268800	2.91106800
C	-2.62433000	6.90441200	2.63361500
H	-1.59117800	6.95692500	2.98140800
C	-4.76926700	5.57237900	2.56969400
H	-5.20850000	6.43172100	2.05834900
H	-4.91739700	4.69264000	1.93553000
H	-5.35042400	5.40066000	3.48675100
C	0.82077500	1.40583800	3.70585800
H	1.21703200	0.82772000	2.86516500
H	1.15524900	2.43922800	3.62189100
H	1.26474100	0.96555800	4.61153400

C	-0.44835100	-1.19942300	4.30079900
H	-0.12683400	-1.03983200	5.33718700
H	-1.07153000	-2.09202700	4.27029400
H	0.43868900	-1.38802300	3.69424600
C	-3.08060300	8.13121700	1.89621400
H	-3.00451600	9.01985000	2.53775000
H	-2.43411500	8.31931800	1.02863100
H	-4.11020800	8.06485900	1.53642700

TS-1-1-6RR-3

l imaginary frequency

H = -5393.903527

G = -5394.110157

E(M06-2X-DCM) = -5394.833894

C	-1.93536500	3.46468600	2.94233300
C	-1.41235400	2.50477200	4.08427100
H	-2.27570500	2.24219400	4.70058300
H	-0.75151700	3.12160600	4.70670700
C	-0.64032100	1.24423300	3.80417700
C	-0.76844800	4.10486900	2.16781300
H	-1.15865700	4.90565300	1.53068600
H	-0.09085300	4.59134100	2.87637900
N	0.01240200	3.17786700	1.36022100
C	1.14585400	3.56737600	0.69978100
N	1.64349200	2.56470900	-0.09360500
C	2.68753900	2.52952500	-1.02661100
C	3.74752500	3.44249700	-1.10984000
C	2.64700200	1.44958300	-1.93188300
C	4.73517800	3.26626700	-2.08490500
C	3.63584700	1.29862500	-2.89425900
H	1.82248100	0.74735600	-1.88495600
C	4.69613400	2.20604100	-2.98427100
H	5.46303100	2.09253100	-3.74132700
C	3.56261200	0.17199800	-3.88664800
C	5.89892700	4.22441500	-2.10307300
F	2.45914600	-0.59613200	-3.71529200
F	3.52467200	0.63352400	-5.15937400
F	4.63337500	-0.65309100	-3.80705000
F	6.55928900	4.19722100	-3.28214800
F	5.50728900	5.49646700	-1.88518900
F	6.80014200	3.92035100	-1.13843800
S	1.79747300	5.11004600	0.89433300
C	-2.65617300	4.62614900	3.74428600
H	-1.95736100	4.97358700	4.51759800

H	-3.49781500	4.16313700	4.27063300
H	3.78661800	4.28440600	-0.43302600
C	-1.26036400	-0.01565700	3.80532800
H	1.15214700	1.66943800	-0.01726900
H	-2.30845900	-0.00689100	4.10907100
H	-0.43223600	2.31377400	1.06426700
H	-1.41475100	-0.37460600	2.56679200
O	0.44864200	-2.52675900	0.59458600
O	-0.75905500	-1.16535800	-1.30057500
P	-0.37292300	-1.14974600	0.28058800
O	0.40993400	0.09851900	0.52306300
C	4.19582900	-3.03446200	-1.22914500
C	3.02442100	-3.34094400	-1.91107100
C	1.77787900	-3.24371700	-1.27333000
C	2.88367300	-2.51540500	0.77388900
C	4.11556800	-2.66738500	0.11161000
C	-1.37830600	-2.17050800	-2.06569300
C	-0.76492400	-3.41624700	-2.21870700
C	-1.51192800	-4.48328000	-2.74497000
C	-2.76550800	-4.26215200	-3.29930600
C	-3.24540400	-2.95733800	-3.36055500
C	-2.58468800	-1.87823700	-2.74251900
H	5.02464500	-2.48361700	0.67608400
H	-4.16828500	-2.75254100	-3.89218700
C	0.69692700	-3.85674900	-2.14781800
C	1.34715700	-3.67505400	-3.56720800
H	0.95173700	-4.38799100	-4.29588000
H	1.12271500	-2.66898200	-3.93374700
H	-0.46443900	-6.14718100	-3.66723500
H	-1.31019300	-6.57683700	-2.18587600
C	1.71287500	-2.74919700	0.02565400
H	5.16165500	-3.10257700	-1.72225100
H	-3.33912400	-5.07802000	-3.73152700
C	2.86514600	-3.81032700	-3.33739000
H	3.45365000	-3.20662100	-4.03588400
H	3.20106700	-4.85065300	-3.44937800
C	-0.73277300	-5.77919800	-2.66775200
C	0.51732600	-5.38055000	-1.85264400
H	0.32406200	-5.51250900	-0.78234900
H	1.40823100	-5.96180900	-2.11006500
C	-3.14592500	-0.51020500	-2.98323300
C	-4.52652800	-0.26168600	-2.74422700
C	-2.36108500	0.46689300	-3.65846300
C	-5.37756100	-1.18022300	-2.04566400

C	-5.13162400	0.95930700	-3.22809700
C	-2.97154800	1.71213000	-4.07275700
C	-6.72064100	-0.94318100	-1.89872600
H	-4.94007600	-2.06118500	-1.59744900
C	-6.53650900	1.16810200	-3.05488600
C	-4.33708000	1.91695300	-3.86262200
C	-7.31746600	0.23772800	-2.42374400
H	-7.33462600	-1.65976500	-1.35984700
H	-6.96958900	2.08745600	-3.44232000
H	-4.79614900	2.83727000	-4.21892700
H	-8.38488100	0.40408700	-2.30508600
C	2.92897500	-2.22038000	2.24062700
C	3.50827800	-1.01059900	2.69785900
C	2.56274000	-3.22920000	3.16936600
C	3.87298500	0.05600800	1.81252600
C	3.74798100	-0.81935700	4.11131300
C	2.78422600	-3.01202500	4.58229100
C	4.45198400	1.20725300	2.28076100
H	3.67061400	-0.05245000	0.75351600
C	4.36117100	0.39437000	4.55739500
C	3.37736400	-1.82122000	5.01216300
C	4.70886900	1.37855900	3.67135700
H	4.71257000	2.00079700	1.58642500
H	4.54709000	0.51506400	5.62231300
H	3.56338600	-1.67542700	6.07459600
H	5.17509300	2.29506200	4.02204700
C	-0.26789500	1.23474500	-4.67845400
H	0.76774800	1.04460800	-4.94218000
C	-0.98806800	0.27134600	-4.02033400
H	-0.50577700	-0.66723600	-3.78163200
C	-0.86501500	2.47669700	-5.03239200
H	-0.27648700	3.23269000	-5.54467800
C	-2.18210800	2.70042100	-4.74123000
H	-2.66352000	3.63347400	-5.02472300
C	1.66565300	-5.44081600	3.70045600
H	1.24198000	-6.38536600	3.37039400
C	1.86413500	-5.21102300	5.09109900
H	1.58658600	-5.97770400	5.80916800
C	2.41214200	-4.03082800	5.51457700
H	2.58212600	-3.84562900	6.57264300
C	2.00589600	-4.48845600	2.77564600
H	1.85517600	-4.68975100	1.72179000
N	-1.62333800	-1.23274500	1.35206000
S	-2.88732300	-2.25071700	1.48116600

C	-2.19608200	-3.96723600	1.83822600
O	-3.60468200	-1.88242900	2.70356500
O	-3.60244800	-2.44028100	0.22004300
F	-3.20499000	-4.73960400	2.24970300
F	-1.25772900	-3.93652200	2.78958700
F	-1.66984700	-4.49883600	0.72869600
C	-2.96181000	2.76796600	2.04002100
C	-3.94619600	1.92847200	2.58837600
C	-3.02525300	3.02517700	0.66233700
C	-4.94098900	1.35833500	1.79713400
H	-3.95741900	1.71478600	3.65287400
C	-4.02366800	2.46079400	-0.13247400
H	-2.30193300	3.68060300	0.19032500
C	-4.98575200	1.62387100	0.42852700
H	-5.67264200	0.69711800	2.25186500
H	-4.04134200	2.67450000	-1.19603000
H	-5.75517700	1.17934800	-0.19269500
C	-3.15241400	5.83224800	2.95764000
C	-4.35068900	5.78468100	2.35202300
H	-4.91901700	4.85917700	2.44402700
C	-2.25740000	7.05161600	2.98890800
H	-2.65532900	7.88384200	2.40437600
H	-2.13286400	7.40444900	4.02267400
H	-1.24993700	6.83772200	2.61139700
C	0.84421600	1.34443300	3.71182300
H	1.22855600	0.75260700	2.87555500
H	1.19626100	2.37116200	3.61784400
H	1.28096100	0.90490800	4.62140600
C	-0.47628300	-1.23331900	4.31138900
H	-0.15674800	-1.07619000	5.34881900
H	-1.11758100	-2.11301700	4.28110200
H	0.40989000	-1.44199600	3.70995000
C	-5.03497400	6.84663800	1.53951800
H	-5.25895000	6.47105700	0.53198400
H	-5.99931400	7.11912000	1.99018200
H	-4.44650600	7.76108400	1.43141800

TS-1-2-6SS

l imaginary frequency

H = -5393.907175

G = -5394.116368

E(M06-2X-DCM) = -5394.841795

O	-1.76156600	-0.00939800	1.93659600
O	-2.99168900	-1.47011600	0.15478700

P	-1.74190600	-0.45495700	0.37274700
O	-1.92829200	0.84914200	-0.40161800
N	-0.36874900	-1.26153300	0.15107400
S	0.00921700	-2.18306900	-1.09817500
C	-0.18560800	-3.92602300	-0.44667700
F	0.05458000	-4.78975000	-1.43379100
F	0.67786500	-4.15748600	0.55068300
F	-1.42946100	-4.10559400	0.00640500
C	0.55592800	3.81303600	-0.33009800
C	0.94815800	3.50998500	-1.80503600
H	0.60920800	4.34138100	-2.43733200
H	2.03925700	3.52520100	-1.84400400
C	0.47200500	2.24449200	-2.47860000
C	0.99118800	2.58214400	0.57295400
H	0.10799300	2.13903200	1.02933100
H	1.63953500	2.93844800	1.37565300
N	1.65975000	1.46139100	-0.09851900
C	3.02164700	1.32264300	-0.24110100
N	3.36801700	0.06866900	-0.66952300
C	4.62506000	-0.51795700	-0.92185000
C	5.78923000	0.18264100	-1.26892000
C	4.67079200	-1.91889100	-0.85130700
C	6.97324600	-0.51930800	-1.50046300
C	5.86570700	-2.59833700	-1.07042300
H	3.76973100	-2.47194800	-0.61134400
C	7.03311100	-1.90825600	-1.39279700
H	7.96359900	-2.43780400	-1.55447300
C	5.88694600	-4.08694600	-0.85532200
C	8.19788000	0.24034700	-1.94067500
F	5.83953400	-4.39039300	0.47110600
F	7.00248300	-4.66228600	-1.34905000
F	4.82509400	-4.69563800	-1.42365300
F	9.33731400	-0.38699200	-1.57027300
F	8.23484600	1.48719000	-1.42645200
F	8.24321000	0.36920500	-3.28845600
S	4.09707100	2.58639000	0.04908600
C	1.39752800	5.05955700	0.17194700
H	1.09403600	5.21733000	1.21334900
H	2.44415600	4.74010700	0.19506800
H	5.77472500	1.26004300	-1.33699800
C	-0.86759100	1.86855000	-2.57140800
H	2.60640800	-0.60954400	-0.75299600
H	-1.57986900	2.66760100	-2.34984000
O	1.46020100	-2.04574300	-1.35403200

H	1. 13177500	0. 59027200	-0. 06157700
O	-0. 89855100	-2. 10220000	-2. 24853000
H	-1. 21094600	1. 27482800	-1. 40637300
C	-6. 86129200	0. 02697400	0. 81771400
C	-6. 05186100	-0. 35041900	1. 88272000
C	-4. 79963700	-0. 93929200	1. 65147600
C	-5. 13237200	-0. 71982100	-0. 75503700
C	-6. 41350500	-0. 20337900	-0. 48025400
C	-1. 66606500	-0. 97392900	2. 95874700
C	-2. 79602300	-1. 72141700	3. 29250100
C	-2. 67153900	-2. 79022400	4. 19486000
C	-1. 46823500	-3. 03395500	4. 84490100
C	-0. 39202700	-2. 18584500	4. 60181500
C	-0. 45330700	-1. 14616500	3. 65521600
H	-7. 05785800	0. 03250200	-1. 32119900
H	0. 53813800	-2. 32657900	5. 14307200
C	-4. 26800400	-1. 52215300	2. 95269100
C	-4. 95352400	-0. 56822100	3. 98829600
H	-5. 02038500	-1. 01362400	4. 98542000
H	-4. 35681800	0. 34757200	4. 07118800
H	-3. 84103500	-4. 62852900	4. 26572600
H	-4. 45956000	-3. 33798300	5. 29012300
C	-4. 31372600	-1. 02730200	0. 34843900
H	-7. 83930600	0. 46967300	0. 98843300
H	-1. 37066200	-3. 85498500	5. 55047000
C	-6. 32815500	-0. 24280400	3. 36622000
H	-7. 09356000	-0. 96532600	3. 68170500
H	-6. 69755300	0. 74877500	3. 65206100
C	-3. 97682500	-3. 54261300	4. 32432300
C	-4. 80274300	-2. 98130700	3. 14975100
H	-5. 88298000	-3. 00989300	3. 32094100
H	-4. 59343900	-3. 55710100	2. 24085400
C	0. 74666900	-0. 25999700	3. 54218500
C	0. 67436400	1. 08270400	3. 99444400
C	1. 99659100	-0. 81942600	3. 17439300
C	-0. 54185100	1. 69734500	4. 43770000
C	1. 88111400	1. 87735500	4. 06091000
C	3. 19867300	-0. 02535200	3. 28969400
C	-0. 57207600	2. 99864500	4. 87015900
H	-1. 45507000	1. 11383200	4. 44069800
C	1. 80421600	3. 23489800	4. 50669200
C	3. 10710000	1. 30193400	3. 71600500
C	0. 61378300	3. 78720100	4. 89593300
H	-1. 51008500	3. 43327700	5. 20598800

H	2. 72215100	3. 81689200	4. 53545500
H	4. 01232300	1. 90035400	3. 78333100
H	0. 56971200	4. 81782700	5. 23694200
C	-4. 77883900	-0. 96878100	-2. 18534500
C	-4. 55300900	-2. 29139200	-2. 64605600
C	-4. 82792400	0. 10735900	-3. 10795800
C	-4. 52398900	-3. 43066000	-1. 77965300
C	-4. 37842600	-2. 53096400	-4. 06110700
C	-4. 70069700	-0. 15722400	-4. 52362000
C	-4. 29426800	-4. 69212600	-2. 26240900
H	-4. 69083000	-3. 29132900	-0. 71863400
C	-4. 13799900	-3. 86227800	-4. 52403900
C	-4. 47614500	-1. 46523100	-4. 95914700
C	-4. 08880000	-4. 91550100	-3. 65284400
H	-4. 27095900	-5. 53486500	-1. 57680600
H	-3. 99677700	-4. 01660200	-5. 59106700
H	-4. 37058800	-1. 65899800	-6. 02467500
H	-3. 90206600	-5. 92237900	-4. 01575500
C	3. 36411900	-2. 69023800	2. 39798700
H	3. 44195100	-3. 70657100	2. 02183200
C	2. 13364400	-2. 16092300	2. 69000300
H	1. 24246200	-2. 75516600	2. 53598100
C	4. 54936500	-1. 91646400	2. 55709200
H	5. 51016400	-2. 35951900	2. 31450900
C	4. 46290500	-0. 61680500	2. 97621400
H	5. 35438200	-0. 00270800	3. 07329900
C	-5. 02482500	2. 49159900	-3. 62116000
H	-5. 11823500	3. 51919500	-3. 27998400
C	-4. 95084300	2. 21787900	-5. 01682600
H	-5. 01042400	3. 03470600	-5. 73105600
C	-4. 78558800	0. 92995800	-5. 44955900
H	-4. 70448700	0. 70705200	-6. 51090800
C	-4. 96651000	1. 47586200	-2. 70166500
H	-4. 99567000	1. 70912600	-1. 64369700
C	-0. 93025400	4. 17302600	-0. 13072000
C	-1. 68907900	4. 80053100	-1. 13222800
C	-1. 54198900	4. 01451200	1. 12413700
C	-3. 00721400	5. 20510000	-0. 91101100
H	-1. 25624800	4. 99261300	-2. 10837100
C	-2. 85670300	4. 42160300	1. 35300000
H	-0. 99583800	3. 57618400	1. 95295400
C	-3. 60295800	5. 01309200	0. 33449200
H	-3. 56123300	5. 68126900	-1. 71622900
H	-3. 29500300	4. 27138800	2. 33618600

H	-4.62817400	5.32728900	0.51080100
C	1.28715200	6.37523400	-0.58349800
C	0.35657800	7.27760300	-0.22819400
H	-0.30907100	7.00595700	0.59139400
C	-1.32325900	0.88207600	-3.63948600
H	-1.19146700	1.30935000	-4.64280100
H	-0.79039400	-0.06995600	-3.59704700
H	-2.38015800	0.66177800	-3.50740300
C	0.08840800	8.63768400	-0.80837700
H	-0.94718500	8.70344600	-1.16978500
H	0.19792000	9.41705200	-0.04149500
H	0.74779400	8.89612700	-1.64098600
C	1.50255300	1.46294600	-3.23962000
H	2.52346300	1.73527500	-2.97101300
H	1.37120200	0.38284500	-3.11637700
H	1.36064200	1.66141400	-4.31329900
C	2.33285600	6.61923700	-1.65048900
H	3.33944200	6.55219100	-1.21630900
H	2.29794500	5.86819800	-2.44916600
H	2.23925200	7.60080800	-2.12086300

TS-1-2-6SS-1

l imaginary frequency

H = -5393.904964

G = -5394.115235

E(M06-2X-DCM) = -5394.838806

O	-1.89613300	0.58415000	1.87153700
O	-3.09620500	-1.23188700	0.42510900
P	-1.87745200	-0.15428900	0.42466100
O	-2.09189400	0.96771300	-0.58639100
N	-0.49248200	-0.97434100	0.34741800
S	-0.14609700	-2.19203900	-0.61883300
C	-0.41629600	-3.72217600	0.42781100
F	-0.23585400	-4.80615700	-0.32743100
F	0.46010600	-3.74795000	1.44045700
F	-1.65473700	-3.73497000	0.92945400
C	1.01675800	3.58423400	-1.65128500
C	1.10313000	2.69628000	-2.93846600
H	0.82352000	3.32236400	-3.79723600
H	2.15800400	2.44628900	-3.07542100
C	0.28236000	1.44220600	-3.09510400
C	1.40217500	2.68800600	-0.40773600
H	0.50567900	2.47542100	0.17275400
H	2.09908100	3.22146800	0.23830300

N	1. 95551400	1. 35942000	-0. 69433200
C	3. 29278400	1. 06215600	-0. 81666500
N	3. 50556300	-0. 28906800	-0. 91006300
C	4. 68723600	-1. 05577700	-0. 93539800
C	5. 95034300	-0. 59149000	-1. 33136300
C	4. 54661300	-2. 40131600	-0. 55801100
C	7. 04219000	-1. 46082900	-1. 30830800
C	5. 65153300	-3. 24713900	-0. 52944600
H	3. 56970000	-2. 77877600	-0. 27583400
C	6. 91459600	-2. 78781600	-0. 89906300
H	7. 77459300	-3. 44477500	-0. 86855900
C	5. 45845900	-4. 64721500	-0. 01320400
C	8. 37792700	-0. 96598800	-1. 80059700
F	5. 22799900	-4. 64760200	1. 32670500
F	6. 53742300	-5. 42789600	-0. 22763100
F	4. 39530300	-5. 25239700	-0. 58454500
F	9. 40353000	-1. 62688200	-1. 21665500
F	8. 55291700	0. 34975200	-1. 55924700
F	8. 50974400	-1. 14230000	-3. 13697100
S	4. 48740900	2. 24702200	-0. 87604500
C	2. 07911700	4. 73231300	-1. 91704300
H	3. 06835000	4. 26574100	-1. 86288700
H	1. 93294700	5. 05882900	-2. 95315000
H	6. 07919800	0. 43702700	-1. 63348400
C	-1. 10751100	1. 42856400	-2. 97518800
H	2. 67242500	-0. 87505900	-0. 81680800
H	-1. 56248400	2. 42025900	-2. 92570900
O	1. 31249100	-2. 19718200	-0. 86302600
H	1. 35793000	0. 59309200	-0. 39003000
O	-1. 02544400	-2. 35071500	-1. 78571100
H	-1. 38349500	1. 13851800	-1. 70925500
C	-7. 05521400	0. 05898000	0. 98683500
C	-6. 17351000	-0. 01990800	2. 05815600
C	-4. 88544400	-0. 54847700	1. 88302600
C	-5. 33000200	-0. 86474600	-0. 49485700
C	-6. 64206300	-0. 41039000	-0. 25678400
C	-1. 71493600	-0. 16216800	3. 05095000
C	-2. 78755100	-0. 89077600	3. 56349400
C	-2. 57343300	-1. 76046200	4. 64521400
C	-1. 33905400	-1. 81238300	5. 28026200
C	-0. 32227700	-0. 97114600	4. 83830200
C	-0. 47362100	-0. 13602600	3. 71572400
H	-7. 34222600	-0. 42072400	-1. 08588600
H	0. 62999200	-0. 95741000	5. 35869800

C	-4.27659600	-0.83856100	3.24836500
C	-4.99149700	0.25379900	4.11226800
H	-4.99485600	0.00691200	5.17810900
H	-4.45696700	1.20315400	3.99141400
H	-3.62877800	-3.61082400	5.10879800
H	-4.29618600	-2.18217700	5.89080000
C	-4.43970000	-0.85814500	0.59853400
H	-8.06221100	0.44657100	1.11862000
H	-1.17208600	-2.47775600	6.12336500
C	-6.40504000	0.36600100	3.50260600
H	-7.10983000	-0.32156500	3.99020600
H	-6.82976700	1.37153600	3.60277500
C	-3.82729300	-2.54271600	4.96457400
C	-4.71495500	-2.26211800	3.73593100
H	-5.78684600	-2.31941800	3.94714200
H	-4.49090500	-2.98693600	2.94469400
C	0.66429700	0.77799700	3.39018900
C	0.51389000	2.17736700	3.57445100
C	1.94159900	0.23015600	3.10828100
C	-0.73546700	2.79653800	3.90512400
C	1.67422200	3.03550700	3.48103900
C	3.09430500	1.09985400	3.04339400
C	-0.83768300	4.15021000	4.09834200
H	-1.61727900	2.17710900	4.01513400
C	1.52514400	4.44250200	3.69435000
C	2.92882300	2.47531800	3.22343700
C	0.30596500	4.99090300	3.98877200
H	-1.80031700	4.58705300	4.35094500
H	2.41208900	5.06734300	3.62498300
H	3.80059700	3.12392400	3.17513200
H	0.20787700	6.06072500	4.15077200
C	-5.01447800	-1.39171000	-1.85736400
C	-4.64008800	-2.75025700	-2.02976400
C	-5.23698800	-0.56760300	-2.99122700
C	-4.45951200	-3.66041900	-0.93978700
C	-4.46606300	-3.27734000	-3.36479700
C	-5.10368000	-1.12477600	-4.31862300
C	-4.08681200	-4.96256100	-1.14633100
H	-4.62675100	-3.31253800	0.07183100
C	-4.07165400	-4.64080000	-3.53793300
C	-4.71412200	-2.45754700	-4.46813900
C	-3.87810400	-5.46254500	-2.46205900
H	-3.94988000	-5.62394100	-0.29522000
H	-3.93313300	-5.00973800	-4.55135600

H	-4.60383400	-2.86901000	-5.46946400
H	-3.57565400	-6.49615500	-2.60517200
C	3.41463900	-1.67591200	2.69092400
H	3.55417300	-2.74051800	2.52524500
C	2.15600700	-1.17103800	2.89323700
H	1.30130600	-1.83510300	2.87514500
C	4.55029800	-0.81630700	2.66760300
H	5.53771300	-1.23747000	2.50334800
C	4.38902100	0.53335700	2.82167300
H	5.24219300	1.20462300	2.77479700
C	-5.78917000	1.58919900	-4.01122200
H	-6.02884600	2.64361600	-3.90243800
C	-5.69962300	1.02095900	-5.31358500
H	-5.88916700	1.63913200	-6.18687100
C	-5.35703300	-0.29621700	-5.45692900
H	-5.26426600	-0.74111500	-6.44498000
C	-5.56413600	0.82571300	-2.89428900
H	-5.61006600	1.28655300	-1.91466600
C	-0.35678900	4.26993100	-1.48198100
C	-0.96066700	4.90439200	-2.58410200
C	-1.00410400	4.39754000	-0.24464100
C	-2.16407200	5.59659200	-2.46665000
H	-0.48608500	4.86749500	-3.56102000
C	-2.20910900	5.09498800	-0.11991600
H	-0.58434000	3.96567700	0.65616900
C	-2.80117400	5.69311300	-1.22812800
H	-2.60083200	6.06421800	-3.34546200
H	-2.67951500	5.16211200	0.85727900
H	-3.74039900	6.23091900	-1.13148500
C	2.05864800	5.97258500	-1.04207600
C	1.69019700	7.14697100	-1.58086000
H	1.38238100	7.14205400	-2.62740100
C	-1.94014400	0.37762500	-3.70803400
H	-1.76023000	0.42658700	-4.78971500
H	-1.73627200	-0.64130300	-3.37035200
H	-2.99462900	0.58160600	-3.53392700
C	1.62762900	8.50032000	-0.93102300
H	2.22366400	9.23254500	-1.49287800
H	0.59539700	8.87758200	-0.92505900
H	1.98278300	8.50227200	0.10273000
C	0.99708800	0.22723400	-3.59682700
H	2.05118000	0.21394900	-3.31673200
H	0.51550100	-0.70303900	-3.28519400
H	0.94355100	0.24858500	-4.69827300

C	2. 52393900	5. 81924100	0. 38664600
H	1. 74988200	5. 36486400	1. 01851400
H	3. 40541200	5. 16879800	0. 43973600
H	2. 78564700	6. 77723800	0. 84384300

TS-1-2-6SS-2

l imaginary frequency

H = -5393.906650

G = -5394.116764

E(M06-2X-DCM) = -5394.841582

O	-1. 99579100	0. 98371300	1. 61525300
O	-3. 13697100	-1. 11288400	0. 55571200
P	-1. 92323800	-0. 04853000	0. 36015700
O	-2. 12168200	0. 82221500	-0. 87605800
N	-0. 53372300	-0. 84877900	0. 50892900
S	-0. 15886500	-2. 23018200	-0. 19303800
C	-0. 47001300	-3. 52759300	1. 12209300
F	-0. 24510800	-4. 73623800	0. 60576900
F	0. 35781600	-3. 33697300	2. 15821100
F	-1. 73025600	-3. 46288400	1. 56081000
C	1. 07910000	3. 32796400	-2. 11759900
C	1. 20604000	2. 28995100	-3. 28871900
H	0. 91698300	2. 80449300	-4. 21606400
H	2. 26715900	2. 04987900	-3. 38433500
C	0. 41919300	1. 00168300	-3. 28581700
C	1. 60058000	2. 66360100	-0. 78761400
H	0. 82969000	2. 66979100	-0. 02171200
H	2. 43041100	3. 25743400	-0. 40394200
N	2. 03633000	1. 26429500	-0. 86756800
C	3. 34537800	0. 87031100	-1. 02216900
N	3. 50922300	-0. 47232200	-0. 80924300
C	4. 66159500	-1. 27806900	-0. 71494000
C	5. 91771800	-0. 97596400	-1. 26224900
C	4. 49725400	-2. 49117100	-0. 02624100
C	6. 97927600	-1. 86436600	-1. 08302000
C	5. 57292700	-3. 35619100	0. 15201400
H	3. 52432100	-2. 74980100	0. 37690800
C	6. 82923100	-3. 05311200	-0. 36937000
H	7. 66735400	-3. 72228500	-0. 22198300
C	5. 35180500	-4. 59442900	0. 97804600
C	8. 30378100	-1. 55706800	-1. 73313100
F	5. 08381500	-4. 27810700	2. 27247900
F	6. 42731000	-5. 40846800	0. 98393300
F	4. 29808600	-5. 31298800	0. 53430200

F	9.33554700	-2.10739600	-1.05315800
F	8.53398000	-0.23025700	-1.81590300
F	8.36204800	-2.04631600	-2.99471500
S	4.56491100	1.94254700	-1.47516600
C	2.06818200	4.49592900	-2.52242000
H	3.03430500	4.02539900	-2.72110600
H	1.71146400	4.91444600	-3.47333300
H	6.06525000	-0.05238200	-1.80151000
C	-0.97435100	0.95511700	-3.22609700
H	2.66392300	-0.98696000	-0.55143600
H	-1.46378500	1.92146200	-3.36329700
O	1.30745000	-2.28136800	-0.37542900
H	1.42422300	0.60615500	-0.38939000
O	-0.99591900	-2.61041200	-1.33876600
H	-1.32885700	0.85935200	-1.94249000
C	-7.10892600	0.24523500	0.68122400
C	-6.27371500	0.38416000	1.78357000
C	-4.97976200	-0.15808900	1.76894200
C	-5.32347800	-0.93656500	-0.51815000
C	-6.64302400	-0.45190700	-0.43037800
C	-1.85391800	0.50419900	2.93090000
C	-2.93880000	-0.11628100	3.54947400
C	-2.75358400	-0.74075500	4.79402300
C	-1.54036000	-0.64428500	5.46384600
C	-0.51440900	0.10079800	4.88935900
C	-0.63534500	0.68337500	3.61465300
H	-7.30541700	-0.62359800	-1.27282400
H	0.42060200	0.23380300	5.42426100
C	-4.41770100	-0.15418600	3.18404400
C	-5.17168100	1.08158700	3.78095300
H	-5.21314200	1.05777800	4.87400000
H	-4.63921000	1.99372000	3.48727100
H	-3.80719200	-2.47230000	5.59610500
H	-4.51401600	-0.92423300	6.04512600
C	-4.48357400	-0.71605400	0.59191100
H	-8.11998500	0.64437800	0.69219000
H	-1.39698800	-1.12003200	6.43054800
C	-6.56248800	1.04799400	3.11209000
H	-7.27892100	0.46072000	3.70297100
H	-6.99903300	2.04652600	2.99435700
C	-4.01065400	-1.46016600	5.22838500
C	-4.85876000	-1.45334800	3.94097100
H	-5.93661800	-1.48321500	4.12610000
H	-4.60107900	-2.32191500	3.32393800

C	0.50341000	1.52495900	3.13434400
C	0.33431500	2.92962200	3.01786800
C	1.79022700	0.94766300	2.98645300
C	-0.92540200	3.58696200	3.20632900
C	1.48227100	3.76429300	2.74038700
C	2.93288800	1.80109800	2.74865800
C	-1.04945900	4.94725000	3.08696400
H	-1.79557800	2.99350100	3.46039900
C	1.30798300	5.17867700	2.61576800
C	2.74715500	3.18039600	2.62526800
C	0.07880700	5.75838800	2.77710000
H	-2.01845400	5.41537900	3.23928800
H	2.18240600	5.78489400	2.39425600
H	3.61021000	3.81593200	2.43964600
H	-0.03947500	6.83418300	2.68237100
C	-4.94121500	-1.70740200	-1.74010600
C	-4.57263300	-3.07403700	-1.63638100
C	-5.08798100	-1.10632900	-3.01700100
C	-4.46408000	-3.76576700	-0.38789300
C	-4.32798300	-3.83896500	-2.83850000
C	-4.88478900	-1.89923500	-4.20872000
C	-4.09511800	-5.08385900	-0.32790300
H	-4.68380000	-3.23530000	0.53026400
C	-3.94006000	-5.21112900	-2.73301800
C	-4.50240500	-3.23695200	-4.08672800
C	-3.81790100	-5.81925500	-1.51417700
H	-4.01425600	-5.57625900	0.63730700
H	-3.74764600	-5.76165300	-3.65074200
H	-4.33920700	-3.82633600	-4.98677700
H	-3.51966700	-6.86170100	-1.44572500
C	3.28956000	-0.98357000	2.98076400
H	3.44318600	-2.05753000	3.04086200
C	2.02329800	-0.46472900	3.06938400
H	1.17690700	-1.12978800	3.18537000
C	4.41462600	-0.13217500	2.78384900
H	5.40833900	-0.56449700	2.71329900
C	4.23614600	1.21824800	2.65639700
H	5.08208600	1.87614600	2.47608800
C	-5.56147200	0.82411800	-4.44683200
H	-5.79737400	1.88011100	-4.54856000
C	-5.40316100	0.02526300	-5.61470700
H	-5.53710400	0.47130400	-6.59645300
C	-5.06488200	-1.29525400	-5.49292200
H	-4.92012700	-1.91461800	-6.37508600

C	-5.40681200	0.28046900	-3.19717300
H	-5.50368100	0.91380500	-2.32329100
C	-0.35783000	3.89893700	-2.03302200
C	-0.92095700	4.48328100	-3.18620600
C	-1.14035800	3.91897300	-0.87120900
C	-2.19529800	5.04482400	-3.18318800
H	-0.35601100	4.50631900	-4.11421700
C	-2.41915500	4.48553300	-0.86054700
H	-0.78433700	3.49867400	0.06038900
C	-2.95675600	5.05056900	-2.01232700
H	-2.59075500	5.48115800	-4.09695000
H	-2.98891400	4.47258000	0.06419400
H	-3.95128600	5.48822200	-2.00294200
C	2.29148500	5.64320700	-1.54791100
C	3.48831600	5.74676000	-0.94171000
H	4.22074500	4.96688900	-1.14813600
C	-1.73270200	-0.23707300	-3.80916200
H	-1.50387900	-0.35837200	-4.87609900
H	-1.50642400	-1.17696400	-3.29942300
H	-2.80160200	-0.05705500	-3.71281600
C	3.97253900	6.81513100	-0.00141100
H	4.29220300	6.37466900	0.95348700
H	4.85652300	7.32235000	-0.41246500
H	3.22182500	7.57814700	0.22041100
C	1.18049900	-0.25723800	-3.56566600
H	2.24383700	-0.16985600	-3.34335200
H	0.76131600	-1.12214900	-3.04272400
H	1.07428600	-0.47590700	-4.64098500
C	1.18284400	6.65961200	-1.38508500
H	0.73096800	6.90124500	-2.35473500
H	0.37206300	6.28332400	-0.75100600
H	1.54156900	7.59337300	-0.94436400

TS-1-2-6SS-3

l imaginary frequency

H = -5393.908460

G = -5394.117590

E(M06-2X-DCM) = -5394.842992

O	-1.77632800	-0.01552700	1.93738500
O	-3.02337100	-1.41918500	0.12175900
P	-1.75826900	-0.42903000	0.36461000
O	-1.92220600	0.89371200	-0.38312200
N	-0.39779700	-1.25314000	0.13116100
S	-0.02738800	-2.14414000	-1.14259200

C	-0.25390400	-3.90181200	-0.54282800
F	-0.02256000	-4.74027900	-1.55354100
F	0.60036700	-4.17638500	0.45153900
F	-1.50283800	-4.07395400	-0.10111400
C	0.59482600	3.81213700	-0.20928600
C	0.99265300	3.54625400	-1.68979200
H	0.69115500	4.41258300	-2.29417700
H	2.08437700	3.53729900	-1.71410000
C	0.50171400	2.31340100	-2.40883000
C	1.02577900	2.55865200	0.66447700
H	0.14253100	2.11773700	1.12337000
H	1.68827000	2.89183400	1.46529600
N	1.67627800	1.44417800	-0.03368300
C	3.03580700	1.29189000	-0.18052000
N	3.36672300	0.04497600	-0.64114000
C	4.61555100	-0.55333200	-0.90563100
C	5.79489200	0.13839000	-1.21762700
C	4.63681600	-1.95669500	-0.88449100
C	6.96862800	-0.57577700	-1.46420100
C	5.82168300	-2.64875500	-1.11760100
H	3.72438700	-2.50231500	-0.67188900
C	7.00375300	-1.96840500	-1.40567500
H	7.92634400	-2.50813400	-1.57838500
C	5.81544400	-4.14409100	-0.95465200
C	8.20980600	0.17817400	-1.86625200
F	5.75186800	-4.49277900	0.35991000
F	6.92497900	-4.72132800	-1.45968900
F	4.74804700	-4.71401900	-1.55209000
F	9.33528100	-0.48613200	-1.51821300
F	8.26785100	1.40091200	-1.29879700
F	8.26441900	0.36390700	-3.20702300
S	4.12611200	2.53527900	0.14263700
C	1.45314200	5.03863900	0.30748300
H	1.25409600	5.11640300	1.38426800
H	2.50197600	4.74569100	0.20658400
H	5.79960200	1.21764200	-1.24683200
C	-0.83994500	1.95157100	-2.52342100
H	2.59557800	-0.61930400	-0.74527800
H	-1.54893900	2.74796100	-2.28476200
O	1.42683900	-2.02281000	-1.38705000
H	1.13494600	0.58073100	-0.02218200
O	-0.92780400	-2.01528600	-2.29440700
H	-1.19698600	1.33066100	-1.37255700
C	-6.87015500	0.13452000	0.78536700

C	-6.07352700	-0.27248400	1.84916100
C	-4.83096100	-0.88059600	1.61583900
C	-5.14578600	-0.61970100	-0.78899400
C	-6.41942300	-0.08537400	-0.51347200
C	-1.70604700	-1.00221900	2.94024600
C	-2.85352700	-1.73130300	3.25471500
C	-2.75636300	-2.81923300	4.13742700
C	-1.56140700	-3.10219700	4.78693700
C	-0.46555000	-2.27403600	4.56377500
C	-0.50031000	-1.21490300	3.63773300
H	-7.05519300	0.17335600	-1.35423000
H	0.45936300	-2.44602000	5.10504100
C	-4.31905200	-1.49495500	2.91048100
C	-4.99156000	-0.54425800	3.95733900
H	-5.07320400	-1.00406500	4.94680800
H	-4.37738600	0.35808300	4.05825000
H	-3.96610500	-4.63243800	4.17149400
H	-4.56124500	-3.34610500	5.21492200
C	-4.33891700	-0.95726400	0.31444600
H	-7.84121600	0.59187100	0.95719300
H	-1.48500100	-3.93861500	5.47686400
C	-6.35594200	-0.18189800	3.33272700
H	-7.13750600	-0.89343200	3.63315700
H	-6.70696200	0.81251300	3.63163300
C	-4.07832000	-3.54495100	4.24799700
C	-4.88575700	-2.94566200	3.07953100
H	-5.96725100	-2.95405100	3.24477100
H	-4.68400900	-3.50994200	2.16175100
C	0.71954700	-0.35342500	3.54743300
C	0.67682400	0.97830500	4.03420700
C	1.95693500	-0.93114600	3.16617200
C	-0.52599800	1.60820700	4.49240000
C	1.90099400	1.74366700	4.12199400
C	3.17629900	-0.16714300	3.30151000
C	-0.52755800	2.89797600	4.95918900
H	-1.45201600	1.04527500	4.47908100
C	1.85400400	3.09034600	4.60341500
C	3.11407700	1.15033800	3.76217300
C	0.67576500	3.65867200	5.00664900
H	-1.45593100	3.34455000	5.30598800
H	2.78479700	3.65050300	4.64825400
H	4.03226200	1.72667200	3.84468800
H	0.65443600	4.68045200	5.37538900
C	-4.78700600	-0.85421000	-2.22041900

C	-4.57593900	-2.17356000	-2.69744600
C	-4.81410800	0.23482000	-3.12878600
C	-4.57151200	-3.32507000	-1.84690000
C	-4.39149800	-2.39622400	-4.11398700
C	-4.67757800	-0.01234200	-4.54674000
C	-4.35484500	-4.58290200	-2.34497400
H	-4.74708700	-3.19824600	-0.78572400
C	-4.16515200	-3.72424200	-4.59316000
C	-4.46610300	-1.31711700	-4.99809000
C	-4.13895300	-4.78999400	-3.73633100
H	-4.35027100	-5.43526100	-1.67098200
H	-4.01589200	-3.86574200	-5.66086600
H	-4.35298600	-1.49771000	-6.06514600
H	-3.96277200	-5.79429500	-4.11145000
C	3.28245500	-2.81120800	2.34121900
H	3.33748500	-3.81884200	1.93856400
C	2.06410800	-2.26265000	2.64814200
H	1.15986800	-2.83280500	2.47986000
C	4.48452800	-2.06816200	2.51920600
H	5.43518900	-2.52583100	2.26421000
C	4.42706500	-0.77828000	2.97222600
H	5.33204300	-0.18697300	3.08471000
C	-4.97841900	2.62785100	-3.61211200
H	-5.06391000	3.65191100	-3.25835600
C	-4.89484900	2.37192000	-5.01057100
H	-4.93835300	3.19877700	-5.71432700
C	-4.74073500	1.08796000	-5.45880600
H	-4.65257200	0.87809000	-6.52224000
C	-4.93987100	1.59948700	-2.70568600
H	-4.97609700	1.81910200	-1.64503100
C	-0.88918900	4.17522300	-0.00535100
C	-1.64346800	4.81625100	-1.00236000
C	-1.50289900	4.00337400	1.24655600
C	-2.95707000	5.23164200	-0.77547000
H	-1.20611700	5.01688800	-1.97487300
C	-2.81466700	4.41793200	1.47913200
H	-0.95979100	3.55045900	2.06946200
C	-3.55462400	5.02991700	0.46809200
H	-3.50713700	5.72230800	-1.57462500
H	-3.25529500	4.25940300	2.45996100
H	-4.57683400	5.35152200	0.64813600
C	1.23257300	6.40180500	-0.33226700
C	1.93908700	6.74922700	-1.42305500
H	2.65357700	6.01942500	-1.80687200

C	-1.29566700	0.99834000	-3.62095700
H	-1.15389600	1.45158000	-4.61147100
H	-0.77030800	0.04144700	-3.60100300
H	-2.35510200	0.78231900	-3.50209800
C	1.91126800	8.04181700	-2.19078700
H	2.88855000	8.54231800	-2.14452300
H	1.70848800	7.86004300	-3.25521400
H	1.16016100	8.74682100	-1.82573100
C	1.52931900	1.54194800	-3.18528500
H	2.55130700	1.79702300	-2.90420600
H	1.38715500	0.46030500	-3.09029400
H	1.39524100	1.76882400	-4.25422000
C	0.28746000	7.33205300	0.39387700
H	-0.68493700	6.86294400	0.57309300
H	0.70151800	7.58369500	1.38099000
H	0.11603100	8.27074400	-0.13848400

TS-1-2-6SR

l imaginary frequency

H = -5393.901943

G = -5394.110116

E(M06-2X-DCM) = -5394.841796

O	-1.85050200	-0.29005600	1.84800600
O	-3.07521900	-1.53499600	-0.09546000
P	-1.78890900	-0.61239800	0.25676600
O	-1.89087200	0.76323100	-0.41803700
N	-0.43327400	-1.41549900	-0.02227700
S	-0.07973900	-2.47163100	-1.16354800
C	-0.07404500	-4.11066400	-0.26056700
F	0.06214200	-5.09691000	-1.14681400
F	0.93956000	-4.17131100	0.61186100
F	-1.22692700	-4.26837200	0.40117600
C	0.50936700	3.70489600	-0.83947900
C	0.78698800	3.20374900	-2.29956100
H	0.32333900	3.92449600	-2.98692000
H	1.86622200	3.26142800	-2.45214400
C	0.32342400	1.84538100	-2.77345500
C	0.92984400	2.57695400	0.19028000
H	0.03826400	2.21073000	0.69769900
H	1.60411100	2.99117000	0.93944900
N	1.56389000	1.37603600	-0.36736500
C	2.92465700	1.23728900	-0.53738200
N	3.27417000	-0.05228500	-0.85342400
C	4.52234500	-0.66832900	-1.06758900

C	5.74248800	-0.00092900	-1.25265100
C	4.50743200	-2.07351700	-1.10935700
C	6.91187100	-0.74006100	-1.44152900
C	5.68719000	-2.78925400	-1.28597300
H	3.56779800	-2.60375700	-1.00007000
C	6.90673100	-2.13362400	-1.45097400
H	7.82253100	-2.69270700	-1.59516100
C	5.62485100	-4.29105200	-1.21746700
C	8.22000500	-0.00340900	-1.57347900
F	5.44276100	-4.71479900	0.06194000
F	6.75629900	-4.87304300	-1.66623900
F	4.59595100	-4.78832700	-1.93571400
F	8.07340900	1.18090100	-2.20399400
F	9.13336600	-0.72183800	-2.26553500
F	8.76553000	0.26014500	-0.36243600
S	3.96096000	2.55431000	-0.41699700
H	5.77461000	1.07826600	-1.24415000
C	-1.01257200	1.44818800	-2.80530900
H	2.50661900	-0.72413000	-0.90282500
H	-1.73603600	2.26210000	-2.71084800
O	1.32861200	-2.25815800	-1.56311100
H	1.04172100	0.51503500	-0.21281900
O	-1.08324100	-2.63174400	-2.21927500
H	-1.29652900	1.02350700	-1.52988300
C	-6.91636900	-0.38253200	1.17757700
C	-6.04549000	-1.04063100	2.03703000
C	-4.78133900	-1.46243000	1.59600000
C	-5.24457200	-0.52365600	-0.60899500
C	-6.51657600	-0.15273200	-0.13499000
C	-1.61136700	-1.35196500	2.74953000
C	-2.59988500	-2.31560300	2.94048700
C	-2.28205600	-3.49925100	3.62456600
C	-1.04989500	-3.64039900	4.25175800
C	-0.14351200	-2.58335300	4.19936900
C	-0.38178100	-1.42660300	3.43345700
H	-7.19395300	0.33624600	-0.82835500
H	0.79510300	-2.65261300	4.73972400
C	-4.10182100	-2.28677900	2.68119400
C	-4.82589900	-1.72329000	3.95570200
H	-4.78617800	-2.41937000	4.79831300
H	-4.32234500	-0.79980500	4.26428300
H	-3.11548200	-5.47635800	3.25288300
H	-3.91489700	-4.59385000	4.54815400
C	-4.37338800	-1.15595400	0.29784700

H	-7.89639700	-0.05776200	1.51727300
H	-0.80184300	-4.54581800	4.79962400
C	-6.25662200	-1.39889000	3.48924200
H	-6.91879100	-2.27063100	3.58771000
H	-6.71763100	-0.58664400	4.06239200
C	-3.43724700	-4.47659900	3.56587200
C	-4.39162100	-3.81591700	2.54447200
H	-5.44533300	-4.05905700	2.71321600
H	-4.12931800	-4.13520200	1.52946000
C	0.63923700	-0.33393000	3.46425700
C	0.31034700	0.91762400	4.04993700
C	1.97569200	-0.60404300	3.07103100
C	-0.98935400	1.22564100	4.56768000
C	1.33584500	1.92665800	4.19791900
C	2.99520200	0.40314700	3.26238500
C	-1.26176600	2.43376400	5.15575200
H	-1.76953300	0.47581800	4.51004300
C	1.00587900	3.18232600	4.79936800
C	2.64465700	1.64471200	3.79690000
C	-0.25549600	3.43427800	5.26735600
H	-2.25644300	2.62992200	5.54716700
H	1.79276000	3.92700600	4.89400900
H	3.41527000	2.40112700	3.92794600
H	-0.49042100	4.38745200	5.73301000
C	-4.97587300	-0.25699300	-2.05813600
C	-5.00877000	-1.32501100	-2.98789700
C	-4.88819500	1.08254600	-2.51126500
C	-5.09863400	-2.69809700	-2.59282700
C	-4.98462500	-1.03500400	-4.40479200
C	-4.87984900	1.35789300	-3.93033100
C	-5.13675700	-3.70507800	-3.52067200
H	-5.13229700	-2.93962800	-1.53677000
C	-5.02708500	-2.11660100	-5.33948500
C	-4.93877300	0.29419400	-4.83536700
C	-5.09751800	-3.41496900	-4.91411000
H	-5.19541700	-4.73911600	-3.19243200
H	-5.00203200	-1.88026000	-6.40059500
H	-4.93990200	0.50528300	-5.90293100
H	-5.12575400	-4.22829100	-5.63384700
C	3.69891600	-2.10991500	2.20680500
H	3.98324300	-3.06627300	1.77700400
C	2.38389700	-1.85323300	2.49831100
H	1.63351000	-2.60396500	2.29051500
C	4.70177100	-1.12382800	2.43150900

H	5. 73664400	-1. 34342500	2. 18608900
C	4. 35251200	0. 10283800	2. 92507300
H	5. 10122800	0. 87633100	3. 07348000
C	-4. 70255000	3. 48363700	-2. 08462900
H	-4. 60636700	4. 30756900	-1. 38280200
C	-4. 71725600	3. 74988400	-3. 48446600
H	-4. 65589700	4. 77572400	-3. 83763500
C	-4. 80211100	2. 71474300	-4. 37685800
H	-4. 80665800	2. 90432000	-5. 44778200
C	-4. 78997800	2. 19757900	-1. 61640200
H	-4. 76183300	2. 00949400	-0. 54946200
C	1. 29895400	5. 01416800	-0. 60831800
C	1. 52452000	5. 48405000	0. 69679600
C	1. 73183100	5. 83372300	-1. 66141300
C	2. 17479000	6. 69264800	0. 93794800
H	1. 18871700	4. 90560100	1. 55101100
C	2. 38183500	7. 04764600	-1. 42635500
H	1. 58270000	5. 53602600	-2. 69333000
C	2. 61196500	7. 48402200	-0. 12425500
H	2. 33803200	7. 01513700	1. 96316300
H	2. 71213500	7. 64676900	-2. 27111600
H	3. 12249600	8. 42519800	0. 06115700
C	-1. 02935900	4. 05587500	-0. 71710100
H	-1. 26711600	4. 67558600	-1. 58949200
H	-1. 59760300	3. 12794400	-0. 81609600
C	-1. 55018300	4. 77626400	0. 51602200
C	-1. 87486500	6. 07711700	0. 42478300
H	-1. 69857400	6. 56887000	-0. 53300100
C	-1. 47375500	0. 30268700	-3. 69795800
H	-0. 82200200	-0. 57032900	-3. 64779400
H	-2. 46909700	-0. 03015800	-3. 40726400
H	-1. 52427500	0. 63274700	-4. 74412600
C	-2. 42084000	6. 98454600	1. 49044800
H	-2. 66622600	6. 46364600	2. 41974100
H	-1. 69117500	7. 76940900	1. 73481100
H	-3. 32660100	7. 49938500	1. 14251600
C	1. 36129800	0. 98317800	-3. 43274800
H	2. 37838900	1. 30732800	-3. 21345800
H	1. 25515500	-0. 07436000	-3. 17215100
H	1. 20718900	1. 04289300	-4. 52140200
C	-1. 73764800	3. 94941400	1. 76674300
H	-2. 16930700	2. 96999400	1. 52874000
H	-0. 78842800	3. 75484200	2. 28194700
H	-2. 39282800	4. 43546900	2. 49403500

TS-1-2-6SR-1

1 imaginary frequency

H = -5393.901673

G = -5394.110387

E(M06-2X-DCM) = -5394.840905

O	-1.79357300	-0.19465400	1.85808200
O	-3.05967000	-1.52827400	0.00208300
P	-1.76049600	-0.60113000	0.28616400
O	-1.86302400	0.73998500	-0.45617900
N	-0.41921900	-1.43576400	0.03663700
S	-0.07961300	-2.46631000	-1.13426500
C	0.05070400	-4.10204900	-0.23555900
F	0.15559100	-5.08294100	-1.13190800
F	1.13095700	-4.12365700	0.55657400
F	-1.04028900	-4.30031300	0.51153100
C	0.44856900	3.73968400	-0.92767000
C	0.79310200	3.20029500	-2.35638900
H	0.35024800	3.89350600	-3.08523500
H	1.87675800	3.26636800	-2.46973900
C	0.35919400	1.82335700	-2.80742100
C	0.89607300	2.67340600	0.15881700
H	0.02331100	2.35318300	0.72905400
H	1.60410800	3.12743500	0.84979500
N	1.51411500	1.44264900	-0.34966500
C	2.87479900	1.28616600	-0.51045600
N	3.21584700	-0.01318600	-0.79166000
C	4.45872400	-0.64065800	-1.00934200
C	5.67993600	0.01620000	-1.22052700
C	4.43535700	-2.04647900	-1.02816700
C	6.84264900	-0.73235000	-1.41470400
C	5.60804900	-2.77149900	-1.21237400
H	3.49540800	-2.56977000	-0.89506700
C	6.82910100	-2.12546300	-1.40466000
H	7.73924100	-2.69205400	-1.55562700
C	5.54354800	-4.27193000	-1.11938400
C	8.15236100	-0.00464400	-1.57650000
F	5.44465200	-4.67918800	0.17494000
F	6.64198500	-4.86470300	-1.63208300
F	4.46891000	-4.77444400	-1.76248100
F	8.00350500	1.16724500	-2.22962100
F	9.05480500	-0.74098000	-2.26399800
F	8.71283300	0.28167000	-0.37752100
S	3.92488600	2.59635400	-0.41963300

H	5.71872300	1.09510000	-1.22907500
C	-0.96642900	1.39347600	-2.84228800
H	2.44249800	-0.67780500	-0.84609800
H	-1.71133200	2.18894800	-2.76135800
O	1.29470800	-2.19241700	-1.61081400
H	0.98299700	0.59161500	-0.17654400
O	-1.13206000	-2.66698200	-2.13372400
H	-1.25849700	0.97967100	-1.55953400
C	-6.87384400	-0.18324200	1.15648000
C	-6.01877500	-0.78102500	2.07414800
C	-4.76821300	-1.27606300	1.67303000
C	-5.20837500	-0.52919100	-0.60901900
C	-6.47175500	-0.08849900	-0.17222000
C	-1.58847800	-1.21171300	2.81735100
C	-2.61834500	-2.11368200	3.07943000
C	-2.34862400	-3.26020900	3.84301800
C	-1.11594900	-3.41865900	4.46512800
C	-0.16029500	-2.41393400	4.33012600
C	-0.35493400	-1.29938100	3.49271200
H	-7.13985800	0.34758600	-0.90841200
H	0.78129600	-2.49202000	4.86405400
C	-4.11906000	-2.03359400	2.82332800
C	-4.81460200	-1.33606600	4.04536800
H	-4.79771700	-1.95847600	4.94459200
H	-4.27534600	-0.40917000	4.27275500
H	-3.28440200	-5.21669800	3.63696100
H	-4.02199400	-4.19333200	4.86335000
C	-4.35181100	-1.09377500	0.35475500
H	-7.84506000	0.19606200	1.46347700
H	-0.90495900	-4.29525900	5.07219400
C	-6.23494600	-0.99995500	3.55348200
H	-6.92959800	-1.83280000	3.73184300
H	-6.66129900	-0.12225200	4.05219700
C	-3.55101600	-4.17976200	3.87089500
C	-4.48296200	-3.55361900	2.80898000
H	-5.54528400	-3.73096400	3.00335500
H	-4.24873900	-3.96290500	1.81964100
C	0.71433000	-0.25450000	3.44651600
C	0.44803000	1.04415600	3.95562300
C	2.03362500	-0.60853400	3.06251600
C	-0.82923000	1.43927800	4.46964500
C	1.51799700	2.01442300	4.02882000
C	3.09930700	0.36060500	3.18554200
C	-1.03956800	2.69125400	4.98701600

H	-1.64051300	0.72088500	4.47242500
C	1.25026300	3.31969300	4.54939900
C	2.80924600	1.64889500	3.63935100
C	0.00877300	3.65409400	5.01850700
H	-2.01665600	2.95155700	5.38515500
H	2.06914700	4.03427300	4.58504400
H	3.61312500	2.37761900	3.71353800
H	-0.17753700	4.64287700	5.42867800
C	-4.92911100	-0.40733000	-2.07482000
C	-4.91731900	-1.56505400	-2.89151100
C	-4.87026800	0.88147900	-2.66233200
C	-4.98383300	-2.89346400	-2.36209300
C	-4.87343300	-1.41970600	-4.33001100
C	-4.85237900	1.01096700	-4.10194700
C	-4.97758500	-3.98945300	-3.18362700
H	-5.03705000	-3.02952400	-1.28838500
C	-4.86758100	-2.59062900	-5.15113700
C	-4.86128800	-0.14076200	-4.89380400
C	-4.91394500	-3.84090600	-4.59813400
H	-5.01972700	-4.98615900	-2.75322400
H	-4.82638500	-2.46137400	-6.23001900
H	-4.85123200	-0.03984400	-5.97727900
H	-4.90573300	-4.72315500	-5.23206400
C	3.67804900	-2.23932900	2.27573500
H	3.91393100	-3.22874200	1.89459200
C	2.37914600	-1.90636100	2.56220200
H	1.59339000	-2.63236500	2.40296600
C	4.72751000	-1.29058500	2.43980500
H	5.74893900	-1.57301900	2.20239200
C	4.43911300	-0.02234400	2.86246600
H	5.22364200	0.72298100	2.96243500
C	-4.76756300	3.31861600	-2.48469800
H	-4.71599100	4.21264900	-1.86921400
C	-4.77912700	3.44041800	-3.90415100
H	-4.75174700	4.42617400	-4.36063600
C	-4.81610300	2.31652200	-4.68529700
H	-4.81425900	2.39451200	-5.77006300
C	-4.81304100	2.08519900	-1.88655300
H	-4.78515200	2.01063400	-0.80577800
C	1.19332300	5.07586800	-0.70606400
C	1.37669700	5.57053300	0.59805600
C	1.64226100	5.88129200	-1.76335200
C	1.99026900	6.79980000	0.83158100
H	1.01654600	5.00470500	1.45050600

C	2.25882600	7.11376900	-1.53356800
H	1.52852200	5.55901700	-2.79243100
C	2.43920700	7.58076200	-0.23387000
H	2.11606200	7.14714700	1.85392600
H	2.60116100	7.70398400	-2.37975500
H	2.92178900	8.53737800	-0.05292400
C	-1.11160200	4.00265600	-0.85042000
H	-1.40179000	4.44584400	-1.81290900
H	-1.60898100	3.03530700	-0.78298300
C	-1.68105200	4.89388800	0.24565800
C	-2.14252800	4.34748000	1.38365300
H	-2.05414900	3.26632000	1.49819500
C	-1.39366800	0.22403600	-3.72107600
H	-0.71633400	-0.62864500	-3.66010500
H	-2.37954100	-0.13420300	-3.42797400
H	-1.45174500	0.53964700	-4.77138100
C	-2.80077400	5.03772000	2.54508900
H	-2.88286300	6.11997200	2.41709000
H	-3.81425100	4.64354000	2.70542100
H	-2.24356600	4.84829700	3.47110000
C	1.42271200	0.97448000	-3.44292400
H	2.43019600	1.32188600	-3.21408600
H	1.33303000	-0.08147300	-3.17036200
H	1.28291900	1.01920200	-4.53420200
C	-1.81878900	6.35825500	-0.10841600
H	-0.88490000	6.76658200	-0.50530500
H	-2.57751000	6.48218800	-0.89583600
H	-2.12089200	6.97834800	0.73866800

TS-1-2-6SR-2

1 imaginary frequency

H = -5393.903344

G = -5394.112083

E(M06-2X-DCM) = -5394.841060

O	-1.83966200	-0.35925900	1.93459800
O	-3.06688300	-1.58244900	-0.01735300
P	-1.81792100	-0.60819200	0.33053100
O	-2.00744300	0.78653300	-0.27554600
N	-0.43745300	-1.34189000	-0.02850900
S	-0.11035000	-2.34770400	-1.22340300
C	-0.10834900	-4.02927900	-0.40161700
F	0.00587200	-4.97404200	-1.33491900
F	0.91876400	-4.13732100	0.45069800
F	-1.25126500	-4.20991500	0.27131400

C	0.54713400	3.72018700	-0.39147900
C	0.74777000	3.39620800	-1.90854600
H	0.27832100	4.19417200	-2.49567100
H	1.82196200	3.45204200	-2.09263800
C	0.25470500	2.10117400	-2.50963800
C	1.01243600	2.47130500	0.47270500
H	0.13960800	2.05922400	0.98278500
H	1.72099300	2.80573600	1.23023400
N	1.60463300	1.33661500	-0.23892200
C	2.95771000	1.20221300	-0.46798100
N	3.28201400	-0.06168200	-0.89081900
C	4.52068600	-0.67616600	-1.15568300
C	5.72747100	-0.00446800	-1.40132700
C	4.50733400	-2.08095900	-1.19327600
C	6.88919600	-0.74005500	-1.64301100
C	5.67962400	-2.79377500	-1.42466100
H	3.57509100	-2.61251800	-1.03661700
C	6.88739800	-2.13398300	-1.64848800
H	7.79723500	-2.69046000	-1.83451400
C	5.62429400	-4.29564000	-1.35275400
C	8.18704100	-0.00050200	-1.84242800
F	5.48646800	-4.71929500	-0.06775900
F	6.74121900	-4.87493500	-1.83941900
F	4.57271600	-4.79610100	-2.03537800
F	8.00482800	1.18314200	-2.46543700
F	9.06484800	-0.71713600	-2.58089700
F	8.79424400	0.26525200	-0.66194900
S	4.01353600	2.49638100	-0.28486500
H	5.75564400	1.07492400	-1.39744100
C	-1.08724800	1.72044200	-2.54625900
H	2.50678600	-0.72399100	-0.95813100
H	-1.79702900	2.52983300	-2.35539500
O	1.29660800	-2.13362100	-1.62797700
H	1.07831000	0.46816400	-0.14594900
O	-1.12485200	-2.44223800	-2.27667600
H	-1.37279200	1.16833900	-1.33666200
C	-6.93399100	-0.58695600	1.30424400
C	-6.02748500	-1.21045400	2.15256100
C	-4.75618400	-1.58859100	1.69286700
C	-5.28216300	-0.66622200	-0.50546400
C	-6.56223800	-0.34701500	-0.01468900
C	-1.56300800	-1.44041700	2.79800400
C	-2.53690800	-2.41762700	2.99646400
C	-2.19259800	-3.60552400	3.66020800

C	-0.94690000	-3.74060800	4.26128100
C	-0.05100700	-2.67593100	4.19852100
C	-0.31581100	-1.51301000	3.44992600
H	-7.26879400	0.11154300	-0.69947200
H	0.89995700	-2.74324200	4.71677400
C	-4.04325300	-2.40518800	2.76250800
C	-4.75836600	-1.86363200	4.05072900
H	-4.68800200	-2.56111400	4.89020000
H	-4.27226700	-0.92918200	4.35426800
H	-3.01111200	-5.58957400	3.29092600
H	-3.79681600	-4.72314300	4.60524700
C	-4.37532600	-1.26201000	0.39151100
H	-7.92092900	-0.29872800	1.65675000
H	-0.67961300	-4.64849900	4.79586100
C	-6.20455000	-1.57405100	3.60822100
H	-6.84391300	-2.46120000	3.71865900
H	-6.67506100	-0.77270600	4.18902700
C	-3.33755300	-4.59501700	3.61552700
C	-4.31559700	-3.93724400	2.61596900
H	-5.36343500	-4.19559000	2.79767400
H	-4.06467200	-4.24320300	1.59393800
C	0.70589800	-0.42121700	3.46217400
C	0.38512300	0.84603700	4.01873500
C	2.04043700	-0.70601300	3.06836100
C	-0.92186700	1.19033900	4.49389200
C	1.42228500	1.84377200	4.16278300
C	3.07186400	0.28779900	3.26424900
C	-1.19498500	2.42755600	5.01704400
H	-1.71161300	0.45057300	4.44614800
C	1.09582200	3.12488100	4.71022800
C	2.73394300	1.53568700	3.79230600
C	-0.17749900	3.41769300	5.11894300
H	-2.19872200	2.65462000	5.36618200
H	1.89278400	3.85892700	4.80387000
H	3.51272100	2.28370800	3.92251000
H	-0.41212800	4.39285800	5.53685700
C	-5.04013600	-0.39121000	-1.95698600
C	-4.96277300	-1.46378100	-2.87930600
C	-5.08579800	0.94766100	-2.42137200
C	-4.91982300	-2.83691900	-2.47691400
C	-4.96311700	-1.18233400	-4.29819500
C	-5.11656300	1.21128600	-3.84241300
C	-4.85080600	-3.84802800	-3.39832200
H	-4.93864700	-3.07615600	-1.42028600

C	-4.88932500	-2.26791800	-5.22631300
C	-5.06104600	0.14044600	-4.73910400
C	-4.83013200	-3.56408800	-4.79326900
H	-4.80927800	-4.88076300	-3.06342700
H	-4.88273700	-2.03605900	-6.28867700
H	-5.08631300	0.34178000	-5.80823000
H	-4.77087000	-4.38036400	-5.50776000
C	3.74320700	-2.21799900	2.17260800
H	4.01421400	-3.16876200	1.72210100
C	2.43284300	-1.95234900	2.47774700
H	1.67327300	-2.69092700	2.25871300
C	4.75859800	-1.24799100	2.40940900
H	5.78976400	-1.47573900	2.15588600
C	4.42531800	-0.02516300	2.92319500
H	5.18270800	0.73856900	3.07752500
C	-5.14003800	3.35890800	-2.01623100
H	-5.12640900	4.19450800	-1.32177600
C	-5.20479700	3.61055700	-3.41721400
H	-5.25853900	4.63392600	-3.77857900
C	-5.18852600	2.56439500	-4.30027600
H	-5.22375900	2.74268900	-5.37254000
C	-5.08523200	2.07519600	-1.53664700
H	-5.01827000	1.90144400	-0.46900600
C	1.37070900	4.97330400	-0.01571000
C	1.49091400	5.32832400	1.33930000
C	1.95025700	5.83418200	-0.95671100
C	2.17502000	6.47546100	1.73478800
H	1.04295900	4.70394700	2.10760000
C	2.63590900	6.98718800	-0.56539000
H	1.89190200	5.61615300	-2.01735600
C	2.75537400	7.31462500	0.78251400
H	2.25282500	6.71409600	2.79268000
H	3.08101000	7.62514700	-1.32466800
H	3.29181200	8.20886100	1.08806900
C	-0.94719900	4.02024800	0.01935600
H	-1.58028100	3.20146200	-0.33691900
H	-0.98050800	3.94644300	1.11184800
C	-1.57124700	5.35524500	-0.36011300
C	-1.93204000	6.20258500	0.61814200
H	-1.72028400	5.89787000	1.64350700
C	-1.57783600	0.67725100	-3.54380200
H	-0.98239400	-0.23757000	-3.53269200
H	-2.60244500	0.39130600	-3.31392600
H	-1.56388100	1.08235100	-4.56458100

C	-2.57860400	7.55421000	0.50440300
H	-2.84640400	7.82697400	-0.51980100
H	-3.48994800	7.60429700	1.11575600
H	-1.90485900	8.33415400	0.88551900
C	1.25773400	1.30156200	-3.28983000
H	2.28614100	1.59340800	-3.07829900
H	1.14747000	0.22450500	-3.12932900
H	1.06283500	1.46760700	-4.36089900
C	-1.80226600	5.64891800	-1.82570000
H	-0.87811000	5.97135400	-2.32415700
H	-2.17208700	4.76504000	-2.36017000
H	-2.53448400	6.44603700	-1.97793500

TS-1-2-6SR-3

l imaginary frequency

H = -5393.904996

G = -5394.114695

E(M06-2X-DCM) = -5394.841573

O	-1.82293800	-0.34776000	1.98731700
O	-3.11219200	-1.47107600	0.01301600
P	-1.83865000	-0.53560900	0.37507100
O	-2.00866700	0.88844800	-0.16808200
N	-0.48354600	-1.28489700	-0.04402900
S	-0.21372400	-2.24643800	-1.29053600
C	-0.25582000	-3.96316400	-0.54532300
F	-0.20217100	-4.86740100	-1.52313300
F	0.78826700	-4.14870000	0.27254800
F	-1.38675600	-4.13189600	0.15022600
C	0.67975600	3.76269600	-0.16093200
C	0.79494700	3.54342700	-1.70427900
H	0.27673100	4.38505400	-2.18499600
H	1.85393000	3.62154100	-1.95455700
C	0.27466500	2.28428800	-2.35806100
C	1.06634000	2.43653400	0.61377200
H	0.16513400	2.03419300	1.08112500
H	1.77696800	2.67374200	1.40479000
N	1.61396400	1.32777400	-0.17184600
C	2.96000400	1.16310300	-0.42107900
N	3.23987400	-0.08472400	-0.91722700
C	4.45665900	-0.72042200	-1.22912700
C	5.67787300	-0.07107600	-1.46342400
C	4.40358200	-2.12102000	-1.33124400
C	6.81499800	-0.82584500	-1.75724300
C	5.55194900	-2.85391200	-1.61439300

H	3.45938400	-2.63366900	-1.18377200
C	6.77423000	-2.21749300	-1.82686600
H	7.66533900	-2.78920800	-2.05301200
C	5.45556600	-4.35540000	-1.61179500
C	8.12982900	-0.11343600	-1.94337400
F	5.32272700	-4.83538100	-0.34610000
F	6.54938400	-4.94157600	-2.14091000
F	4.38158200	-4.79433300	-2.30184000
F	7.97163800	1.10224800	-2.50864700
F	8.97643000	-0.81879000	-2.72777500
F	8.76164500	0.08103300	-0.76187500
S	4.05927500	2.40933900	-0.17557900
H	5.73615600	1.00578400	-1.41036400
C	-1.07085400	1.91587200	-2.38525400
H	2.44447300	-0.71978100	-1.00825200
H	-1.76846700	2.71928500	-2.13632200
O	1.19195800	-2.06190500	-1.71242400
H	1.06165700	0.47190400	-0.11980800
O	-1.24993600	-2.25741800	-2.32638000
H	-1.36459400	1.30729000	-1.20030800
C	-6.94558700	-0.40305300	1.37081300
C	-6.04646900	-1.05100000	2.20885700
C	-4.79056700	-1.46030300	1.73410900
C	-5.31507000	-0.51903600	-0.45684500
C	-6.58323700	-0.17329700	0.04722700
C	-1.57863800	-1.46784200	2.80955300
C	-2.59272300	-2.40561800	2.99790600
C	-2.29244700	-3.62462300	3.62591900
C	-1.04304800	-3.83466500	4.19687200
C	-0.09929400	-2.81191200	4.14390600
C	-0.32513300	-1.61591500	3.43595900
H	-7.28808500	0.29788900	-0.63062200
H	0.85763100	-2.93769300	4.63988500
C	-4.09966700	-2.31947800	2.78452600
C	-4.77894500	-1.76860500	4.08722300
H	-4.72625000	-2.47941100	4.91683600
H	-4.25447800	-0.85725700	4.39707800
H	-3.21142100	-5.56081300	3.23641400
H	-3.93232400	-4.68061800	4.57855400
C	-4.41228300	-1.13203000	0.43279400
H	-7.92190500	-0.09204300	1.73343900
H	-0.80904500	-4.76848100	4.70154300
C	-6.21852000	-1.41955100	3.66423800
H	-6.89079900	-2.28168700	3.77675600

H	-6.65006500	-0.60499700	4.25688600
C	-3.48363400	-4.55749900	3.58329900
C	-4.44418600	-3.83501700	2.61300000
H	-5.50018100	-4.04859800	2.80491000
H	-4.22221500	-4.13116600	1.58137000
C	0.74396900	-0.57069200	3.47031300
C	0.49180100	0.68091200	4.09310600
C	2.05603700	-0.89586300	3.03582600
C	-0.78983700	1.06072800	4.60847200
C	1.57709400	1.62107200	4.26689500
C	3.13553000	0.03996500	3.25629700
C	-0.99538800	2.28017900	5.19991100
H	-1.61472500	0.36242300	4.53612400
C	1.32087900	2.88466100	4.88763500
C	2.86584800	1.27328400	3.85335100
C	0.06987000	3.21437100	5.33529400
H	-1.98163200	2.53558600	5.57811300
H	2.15353400	3.57429700	5.00590000
H	3.68085200	1.97746500	4.00446800
H	-0.11110300	4.17576700	5.80812000
C	-5.07764200	-0.25989700	-1.91146000
C	-4.98523900	-1.34304000	-2.82077800
C	-5.13522000	1.07285900	-2.39299300
C	-4.94196500	-2.71185500	-2.40402600
C	-4.97221300	-1.07797700	-4.24266100
C	-5.15987300	1.31852600	-3.81743000
C	-4.85650600	-3.73243800	-3.31351300
H	-4.97587900	-2.94134500	-1.34575200
C	-4.87922800	-2.17266200	-5.15819600
C	-5.07979000	0.23813400	-4.70032700
C	-4.81778500	-3.46375100	-4.71091100
H	-4.81622800	-4.76134800	-2.96679900
H	-4.86100700	-1.95171800	-6.22273200
H	-5.09679500	0.42636600	-5.77199000
H	-4.74431700	-4.28725000	-5.41571400
C	3.66871800	-2.43779200	2.03208400
H	3.88703300	-3.37677100	1.53116900
C	2.37861100	-2.12932600	2.38000800
H	1.58151500	-2.82219300	2.14547600
C	4.73192500	-1.52630700	2.29081600
H	5.74597000	-1.78737300	2.00273900
C	4.46589500	-0.31624300	2.86996900
H	5.26059100	0.40427600	3.04331500
C	-5.22879200	3.48826600	-2.02024500

H	-5.23208800	4.33263800	-1.33646700
C	-5.29253000	3.72097600	-3.42423900
H	-5.36315400	4.73845200	-3.79928600
C	-5.25177900	2.66410400	-4.29332800
H	-5.28332400	2.82764500	-5.36804700
C	-5.15309100	2.21218500	-1.52361400
H	-5.08595800	2.05429500	-0.45346800
C	1.59731500	4.93238000	0.26395600
C	1.84009500	5.15643700	1.63056600
C	2.13463800	5.85705000	-0.64171800
C	2.60577500	6.23505600	2.06851900
H	1.41815900	4.48927000	2.37689500
C	2.89988700	6.94236700	-0.20752200
H	1.96817600	5.74839600	-1.70725700
C	3.14478500	7.13692600	1.14990100
H	2.77766400	6.37176000	3.13329800
H	3.30576800	7.63462800	-0.94071800
H	3.74356600	7.97826600	1.48797800
C	-0.79087000	4.14348500	0.27546700
H	-1.46125200	3.33914300	-0.03812800
H	-0.80317800	4.12011200	1.37255400
C	-1.34642500	5.48940800	-0.18373900
C	-2.01429600	5.58590400	-1.34724900
H	-2.14863200	4.67657600	-1.93291600
C	-1.59471100	0.93358700	-3.42692800
H	-1.02018100	0.00620400	-3.46757800
H	-2.62289200	0.65903300	-3.19796800
H	-1.58343800	1.38675000	-4.42731200
C	-2.63747100	6.80031400	-1.97945800
H	-2.51154900	7.71107700	-1.38951400
H	-2.20253800	6.98751400	-2.97093000
H	-3.71426300	6.64894400	-2.13852900
C	1.25273400	1.52090900	-3.20379600
H	2.28932200	1.77256600	-2.98000600
H	1.11685400	0.43805300	-3.12561800
H	1.05574900	1.77534300	-4.25729100
C	-1.16806600	6.65291200	0.76634900
H	-1.50284200	6.37015200	1.77336300
H	-0.11851700	6.94913000	0.85768700
H	-1.74027900	7.53318300	0.46467000

TS-1-2-6RS

l imaginary frequency

H = -5393.910228

G = -5394.116355

E(M06-2X-DCM) = -5394.841606

O	-1.51856200	-1.30808400	-1.75133000
O	-3.22002000	-0.43666400	0.02240000
P	-1.63543600	-0.64726300	-0.27417000
O	-1.04195000	0.77319900	-0.25583600
N	-1.07872800	-1.72322600	0.76603000
S	0.48944900	-1.96730900	0.95559700
C	0.65689700	-3.78839500	0.57481200
F	0.21357100	-4.04295800	-0.65659300
F	-0.04808000	-4.51567400	1.45054900
F	1.94472500	-4.12887900	0.66245000
C	0.40922300	4.59717400	0.22460000
C	0.10340800	4.25267400	1.72203400
H	-0.85191600	4.73061100	1.96910400
H	0.88247900	4.73093100	2.32276300
C	0.02102500	2.82181800	2.20276700
C	1.77393800	3.97030900	-0.20011200
H	1.91437500	4.12393900	-1.27465700
H	2.57864700	4.50452800	0.30514800
N	1.97575500	2.55708900	0.10881000
C	3.20785800	2.08360500	0.52791600
N	3.27739200	0.71997000	0.53427300
C	4.38574200	-0.12056300	0.80058600
C	5.33417400	0.12437500	1.80348100
C	4.48495200	-1.28974900	0.03743300
C	6.38030000	-0.77669300	1.99772900
C	5.53621100	-2.18176700	0.24863800
H	3.73455900	-1.50242200	-0.71490000
C	6.49982200	-1.93090500	1.22157400
H	7.32301900	-2.61743900	1.37552100
C	5.62406300	-3.39689400	-0.63285300
C	7.36176500	-0.54154000	3.11626900
F	5.88387500	-3.05402300	-1.92735700
F	6.59979100	-4.24484700	-0.25077500
F	4.46444500	-4.08939800	-0.65300500
F	8.59269100	-1.00992300	2.80602000
F	7.48820200	0.76705100	3.41709400
F	6.98077200	-1.17305300	4.25238900
S	4.45937900	3.10316800	1.01855700
H	5.26177500	1.01208500	2.41368100
C	-1.13904700	2.06331400	2.05995900
H	2.46153700	0.19137500	0.21269600
H	-2.00899300	2.63509100	1.72550700

O	1.31603700	-1.30392600	-0.08745300
H	1.40525000	1.90123400	-0.41964900
O	0.91161600	-1.80898900	2.35112600
H	-0.96173000	1.43166900	0.88680300
C	-5.75777500	-3.77610900	-0.14841400
C	-5.36508800	-3.12517600	-1.31164300
C	-4.57991600	-1.96114500	-1.25786500
C	-4.56348800	-2.10472000	1.18067500
C	-5.38510300	-3.24000700	1.08210100
C	-1.93187800	-0.64475800	-2.91308500
C	-3.29320400	-0.55034300	-3.18535900
C	-3.72384400	0.27258000	-4.23698800
C	-2.79904100	0.85313300	-5.09887800
C	-1.44124300	0.59114000	-4.91192200
C	-0.96683400	-0.14516400	-3.81081100
H	-5.72665800	-3.70478300	2.00211800
H	-0.71781100	0.97104400	-5.62662900
C	-4.47857100	-1.34650800	-2.65167500
C	-4.67677200	-2.62979000	-3.53306600
H	-3.71513800	-3.14950300	-3.61440700
H	-5.01236100	-2.39110900	-4.54647600
H	-5.64932400	-0.18037600	-5.13129100
H	-5.59846100	1.38329400	-4.32807100
C	-4.11767000	-1.51688600	-0.01919100
H	-6.36333100	-4.67764600	-0.19258600
H	-3.12468400	1.47188900	-5.93125200
C	-5.67092300	-3.50198000	-2.74306600
H	-5.53939500	-4.57314900	-2.93317800
H	-6.71141200	-3.26111500	-3.00271700
C	-5.23631700	0.35073400	-4.26286500
C	-5.63809600	-0.33542300	-2.93576700
H	-5.66849500	0.40387400	-2.12679800
H	-6.61685100	-0.82299400	-2.97946300
C	0.49084700	-0.44728700	-3.67399100
C	1.44244800	0.60294300	-3.61330600
C	0.92805100	-1.79837400	-3.69520800
C	1.08433000	1.99076400	-3.64899000
C	2.85203800	0.28649100	-3.53132700
C	2.33544900	-2.09691300	-3.56006200
C	2.03978500	2.97546100	-3.67537500
H	0.03553200	2.26229800	-3.67446900
C	3.81239800	1.34627500	-3.51982700
C	3.25719500	-1.04982600	-3.47710700
C	3.42545100	2.65589200	-3.60794100

H	1. 73581000	4. 01696300	-3. 74786600
H	4. 86497800	1. 08368300	-3. 45068600
H	4. 31525300	-1. 28287700	-3. 38163700
H	4. 16581500	3. 45040800	-3. 61309200
C	-4. 31466300	-1. 54373200	2. 54719900
C	-3. 50932200	-2. 24584200	3. 47526600
C	-5. 02286600	-0. 38242200	2. 94933500
C	-2. 76159600	-3. 41495100	3. 12316900
C	-3. 41690100	-1. 77422500	4. 83928300
C	-4. 90756600	0. 08604900	4. 31239800
C	-2. 00114500	-4. 07710300	4. 05061700
H	-2. 77701600	-3. 75599400	2. 09548300
C	-2. 61631300	-2. 49922600	5. 77654900
C	-4. 11357000	-0. 62356800	5. 21775600
C	-1. 93183900	-3. 62152300	5. 39782000
H	-1. 42662000	-4. 94840100	3. 75151000
H	-2. 56262300	-2. 13315500	6. 79914500
H	-4. 04238200	-0. 27522100	6. 24640200
H	-1. 32246500	-4. 16188400	6. 11693800
C	0. 49928900	-4. 19775400	-3. 89484100
H	-0. 20001900	-5. 01536700	-4. 04857300
C	0. 04181000	-2. 90629500	-3. 88787000
H	-1. 01254000	-2. 71591000	-4. 04967700
C	1. 87933700	-4. 48463600	-3. 70106900
H	2. 22002400	-5. 51617200	-3. 68937200
C	2. 77119800	-3. 45956800	-3. 54391500
H	3. 82879500	-3. 65819300	-3. 40033900
C	-6. 56528900	1. 46247600	2. 49782700
H	-7. 22194300	1. 98986400	1. 81082800
C	-6. 43016200	1. 93048900	3. 83603300
H	-6. 97401900	2. 81525700	4. 15544400
C	-5. 62549200	1. 25617200	4. 71384600
H	-5. 52106400	1. 59418300	5. 74230900
C	-5. 88765200	0. 34882700	2. 07165300
H	-6. 01508600	0. 00253400	1. 05221900
C	1. 14537600	2. 31455800	3. 05112300
H	1. 30726900	1. 23961300	2. 92897300
H	2. 08124000	2. 84972500	2. 88237500
H	0. 85274300	2. 46203400	4. 10396400
C	-1. 45063200	0. 90961000	3. 00976500
H	-0. 65037200	0. 16837900	3. 06889500
H	-1. 63879700	1. 29211400	4. 02092300
H	-2. 35088800	0. 39056500	2. 68145800
C	0. 63375500	6. 12602600	0. 07969600

C	0.58031600	7.03015600	1.15144900
C	0.95497900	6.65459800	-1.18412600
C	0.82719900	8.39349700	0.97073800
H	0.33206300	6.69233500	2.15098400
C	1.20767100	8.01287300	-1.36892600
H	1.01064200	6.00061300	-2.04884000
C	1.14366400	8.89432700	-0.28959700
H	0.77118600	9.06145300	1.82620500
H	1.45532300	8.38023900	-2.36135500
H	1.33868800	9.95379900	-0.42986200
C	-0.72764400	4.11431700	-0.73927800
H	-0.43685600	4.45057400	-1.74439300
H	-0.70871600	3.02243800	-0.78414300
C	-2.16960900	4.55586800	-0.50201400
C	-3.13163100	3.61510300	-0.45607900
H	-2.82167800	2.57503400	-0.54520300
C	-2.46421800	6.03841500	-0.46801100
H	-2.06494700	6.52366200	0.42962200
H	-1.99386200	6.54759900	-1.31816300
H	-3.53595400	6.24508200	-0.50685900
C	-4.61883100	3.79379500	-0.32349300
H	-5.00014200	3.20494300	0.52121400
H	-4.92876500	4.83124000	-0.17507800
H	-5.13251200	3.41647600	-1.21958600

TS-1-2-6RS-1

l imaginary frequency

H = -5393.910365

G = -5394.118021

E(M06-2X-DCM) = -5394.840806

O	-1.62742200	-1.37758300	-1.66981800
O	-3.34502300	-0.40751600	0.03187200
P	-1.75721900	-0.59808500	-0.25178700
O	-1.20358900	0.83292700	-0.35121100
N	-1.16405000	-1.57161400	0.86737600
S	0.40705900	-1.76696100	1.06877200
C	0.61792400	-3.60578100	0.81743000
F	0.19928600	-3.95218700	-0.39989700
F	-0.08361400	-4.28688500	1.73110500
F	1.91185200	-3.91001000	0.94545000
C	0.66034300	4.57397000	0.03232300
C	0.45481300	4.25766700	1.55476200
H	-0.35942500	4.89679500	1.91448400
H	1.36999700	4.56380400	2.06838500

C	0.12200100	2.86329000	2.03431200
C	1.99693600	3.90872700	-0.42885500
H	2.08985800	4.01528400	-1.51488200
H	2.83084900	4.44710100	0.02155800
N	2.17522200	2.50661200	-0.06373900
C	3.37341800	2.02742300	0.43659900
N	3.40878300	0.66294200	0.48765700
C	4.48115800	-0.21095500	0.78097800
C	5.48988300	0.05266100	1.71866400
C	4.48566200	-1.43641500	0.10093600
C	6.49912300	-0.88696600	1.92784500
C	5.50475000	-2.36172300	0.32210400
H	3.69080200	-1.66142500	-0.60142300
C	6.52680000	-2.09475400	1.22976100
H	7.32452300	-2.80886800	1.39133400
C	5.50581100	-3.62794500	-0.48921300
C	7.54315300	-0.62404100	2.98218500
F	5.75949600	-3.37166900	-1.80492800
F	6.44028300	-4.50705600	-0.07614700
F	4.30975100	-4.25416800	-0.45189900
F	8.72468000	-1.20492000	2.67038700
F	7.77094200	0.69376700	3.15565700
F	7.16978900	-1.12209900	4.18500600
S	4.61491400	3.04276600	0.95892900
H	5.49223900	0.98434300	2.26396200
C	-1.14257600	2.30471600	1.85126300
H	2.56833700	0.15656600	0.19461000
H	-1.88735900	3.00240300	1.45726500
O	1.22468100	-1.15923000	-0.01587800
H	1.61854600	1.83956400	-0.59166600
O	0.82486100	-1.50198900	2.45044500
H	-1.03109100	1.55473100	0.73432600
C	-5.84490400	-3.77764900	0.06716500
C	-5.45885600	-3.19555500	-1.13431500
C	-4.68380900	-2.02381600	-1.15258000
C	-4.66625300	-2.01686300	1.29036300
C	-5.47644800	-3.16414100	1.26250900
C	-2.03950200	-0.80294600	-2.87797100
C	-3.39990600	-0.72942700	-3.15979900
C	-3.82854300	0.02515000	-4.26215900
C	-2.90122400	0.55278800	-5.15534000
C	-1.54352100	0.30074800	-4.95100600
C	-1.07240300	-0.36663400	-3.80557900
H	-5.81374200	-3.57457500	2.20956500

H	-0.81879600	0.63290500	-5.68794800
C	-4.58422700	-1.49514900	-2.58122000
C	-4.77431300	-2.83155700	-3.38221600
H	-3.80946800	-3.34936100	-3.43171600
H	-5.11131100	-2.65773100	-4.40829600
H	-5.74978900	-0.48734800	-5.13260300
H	-5.70634700	1.12261000	-4.42609300
C	-4.22614700	-1.50053300	0.05632700
H	-6.44257400	-4.68544400	0.07878900
H	-3.22487900	1.11861500	-6.02534200
C	-5.76273000	-3.66050900	-2.54002000
H	-5.62452300	-4.74034900	-2.66532200
H	-6.80478000	-3.44221700	-2.81307000
C	-5.34133100	0.09713700	-4.29692600
C	-5.74609100	-0.50790100	-2.93138600
H	-5.78287300	0.27932100	-2.16952100
H	-6.72278100	-1.00125500	-2.94950500
C	0.38173400	-0.67717700	-3.64996700
C	1.34794300	0.36069900	-3.65253200
C	0.79996400	-2.03336100	-3.58941300
C	1.00816400	1.74865300	-3.76893300
C	2.75332700	0.03013200	-3.55398800
C	2.20339200	-2.34308200	-3.43885500
C	1.97612000	2.71747000	-3.85598000
H	-0.03745300	2.03102100	-3.80624800
C	3.72785700	1.07569300	-3.61004800
C	3.14004200	-1.30600900	-3.41972700
C	3.35787500	2.38279900	-3.77579800
H	1.68620700	3.75741100	-3.98505600
H	4.77725700	0.80346400	-3.53001100
H	4.19516200	-1.54850100	-3.31422200
H	4.10896200	3.16523100	-3.83299000
C	-4.42256200	-1.36520700	2.61695800
C	-3.60383300	-1.99189800	3.58563000
C	-5.14375400	-0.18813500	2.94241500
C	-2.84293100	-3.17301700	3.30982700
C	-3.51177000	-1.42786200	4.91413400
C	-5.02935000	0.37285000	4.27021700
C	-2.07022300	-3.76153800	4.27597200
H	-2.86010100	-3.58414100	2.30799200
C	-2.69737000	-2.07744800	5.89391300
C	-4.22257900	-0.26380100	5.21770000
C	-2.00024700	-3.21426800	5.58866300
H	-1.48728600	-4.64504200	4.03429800

H	-2.64386900	-1.64230100	6.88911700
H	-4.15160200	0.15434300	6.22004300
H	-1.38100700	-3.69705000	6.33963300
C	0.33713300	-4.43447200	-3.64248900
H	-0.37410000	-5.24981800	-3.74503900
C	-0.10210000	-3.13853100	-3.71267700
H	-1.15410100	-2.94376700	-3.88387400
C	1.71371600	-4.72852300	-3.43619800
H	2.04042800	-5.76214200	-3.36444000
C	2.62021400	-3.70843100	-3.34338500
H	3.67549800	-3.91354400	-3.19326500
C	-6.69771300	1.61157400	2.36819400
H	-7.35185100	2.09179700	1.64520500
C	-6.56622200	2.16885600	3.67167200
H	-7.11532400	3.06998400	3.93092400
C	-5.75702100	1.56092800	4.59300400
H	-5.65447200	1.96868700	5.59608100
C	-6.01502000	0.47550100	2.01863700
H	-6.13833700	0.06197000	1.02407400
C	1.12139500	2.18575200	2.91951100
H	1.11824800	1.09719000	2.80507300
H	2.13296200	2.57137600	2.78323900
H	0.82301700	2.38095500	3.96291800
C	-1.69280500	1.27191100	2.83450600
H	-1.01765800	0.42888700	2.99540800
H	-1.88921400	1.74374100	3.80551600
H	-2.63792200	0.87259300	2.46581700
C	0.90474100	6.09178300	-0.16662400
C	1.16798600	6.97474400	0.89269500
C	0.95245600	6.62195900	-1.46781100
C	1.44929500	8.32394100	0.66507000
H	1.15363400	6.62794100	1.91958000
C	1.23822500	7.96639100	-1.70002700
H	0.76024200	5.98288000	-2.32359100
C	1.48671500	8.82904100	-0.63248300
H	1.64273800	8.97689600	1.51203000
H	1.26392700	8.33843000	-2.72093100
H	1.70736600	9.87784700	-0.81032100
C	-0.50199500	4.06444100	-0.86183400
H	-0.21471800	4.24451400	-1.90729700
H	-0.53129900	2.97241600	-0.79854900
C	-1.93242200	4.56775400	-0.70286400
C	-2.29088000	5.62520500	0.04397200
H	-1.51039600	6.17303300	0.56549900

C	-2.90279400	3.75312400	-1.53126000
H	-2.59533300	3.74847600	-2.58671300
H	-2.90922800	2.70478000	-1.20903600
H	-3.92608400	4.13117600	-1.48851300
C	-3.66494600	6.20627400	0.24033100
H	-3.69900400	7.24412500	-0.11878000
H	-4.45370800	5.65038600	-0.27192400
H	-3.92268200	6.23986900	1.30766100

TS-1-2-6RS-2

l imaginary frequency

H = -5393.905573

G = -5394.113467

E(M06-2X-DCM) = -5394.839138

O	-1.31118700	-1.38680400	-1.70708900
O	-3.12008100	-0.55696600	-0.01393200
P	-1.52986600	-0.79600400	-0.21445000
O	-0.91933100	0.61925900	-0.08076700
N	-1.05832100	-1.91851400	0.81605900
S	0.49528000	-2.20294100	1.08072600
C	0.64969000	-4.00864600	0.62865500
F	0.24112100	-4.20673200	-0.62480600
F	-0.09390000	-4.75669700	1.45282600
F	1.92868000	-4.37277500	0.74234300
C	-0.14425700	4.41935100	0.52681200
C	0.04095400	3.98952800	2.02980400
H	-0.73985300	4.48699000	2.61739900
H	0.99664000	4.41092400	2.35523600
C	-0.00448500	2.53500000	2.44944200
C	1.06349800	3.84022900	-0.27151000
H	0.84855300	3.84073100	-1.34232700
H	1.93511900	4.47035300	-0.10333200
N	1.50185000	2.49801300	0.11134300
C	2.81713700	2.22115100	0.43333300
N	3.07495600	0.88029700	0.51395300
C	4.28476000	0.19811800	0.79415900
C	5.28268900	0.67380800	1.65610300
C	4.44131900	-1.06465500	0.20522900
C	6.42316500	-0.09677400	1.88549100
C	5.58443100	-1.82249000	0.45178400
H	3.65960900	-1.46002800	-0.43064300
C	6.59287300	-1.34455500	1.28603500
H	7.48468200	-1.93051100	1.47058500
C	5.73206000	-3.14743900	-0.24619900

C	7.45652300	0.39715800	2.86438800
F	6.08622500	-2.98904700	-1.55440700
F	6.68168100	-3.92121400	0.31812300
F	4.57871500	-3.84836900	-0.24993700
F	8.69239400	-0.06195700	2.56158100
F	7.52052700	1.74427700	2.89973600
F	7.18474500	-0.01709000	4.12514200
S	3.94988400	3.43418800	0.74716300
H	5.17789800	1.63789700	2.13013000
C	-1.14298500	1.74323000	2.32090300
H	2.32255000	0.23567400	0.26066200
H	-2.05201800	2.27797600	2.04033200
O	1.38287500	-1.50235700	0.11755500
H	0.94693800	1.72666800	-0.25450800
O	0.84005900	-2.12135500	2.50315600
H	-0.93299100	1.17325100	1.08693100
C	-5.72846300	-3.81177500	-0.46722400
C	-5.24532400	-3.13124000	-1.57843200
C	-4.43284800	-1.99462400	-1.43063000
C	-4.56698000	-2.23262500	0.99761000
C	-5.41486100	-3.33631500	0.80408300
C	-1.64367800	-0.69238000	-2.87872900
C	-2.98604300	-0.55145800	-3.22191500
C	-3.33330400	0.31047300	-4.27360000
C	-2.34648200	0.87682300	-5.07376000
C	-1.01070500	0.55805100	-4.82814900
C	-0.61637600	-0.21639800	-3.72088700
H	-5.82340400	-3.82692100	1.68234700
H	-0.24018500	0.92014600	-5.50143700
C	-4.22475600	-1.33080400	-2.78878800
C	-4.40232200	-2.57423100	-3.73051200
H	-3.45274500	-3.12025700	-3.77107400
H	-4.66473500	-2.28803100	-4.75306500
H	-5.21811900	-0.04603300	-5.28954500
H	-5.16254200	1.48601800	-4.42750900
C	-4.03784000	-1.61223600	-0.14998300
H	-6.35693300	-4.69096600	-0.58327500
H	-2.60790700	1.52347900	-5.90757700
C	-5.46992600	-3.44423300	-3.03986300
H	-5.35739500	-4.51102400	-3.26372400
H	-6.48421200	-3.16120800	-3.35471800
C	-4.83848700	0.43993600	-4.38046400
C	-5.33662200	-0.27685300	-3.10375300
H	-5.39438600	0.43537900	-2.27259100

H	-6.32391900	-0.73390800	-3.22136800
C	0.82273900	-0.57943400	-3.53487500
C	1.81611900	0.43043900	-3.43995700
C	1.20526600	-1.94793300	-3.55010300
C	1.52255500	1.83282900	-3.47300400
C	3.20734600	0.05517600	-3.31370500
C	2.59390700	-2.30377200	-3.36732300
C	2.51685800	2.77707400	-3.43236900
H	0.48955900	2.15054200	-3.54497300
C	4.21090500	1.07187400	-3.24919000
C	3.55469300	-1.29624000	-3.25328000
C	3.88337000	2.39827100	-3.31691300
H	2.25932900	3.83195100	-3.47991800
H	5.24754700	0.76148400	-3.14610600
H	4.59721800	-1.57132300	-3.11631000
H	4.65394800	3.16137200	-3.26677500
C	-4.36780300	-1.74293000	2.39850100
C	-3.66724300	-2.53770100	3.33762800
C	-5.01650900	-0.55126400	2.81212900
C	-2.96347400	-3.72999100	2.97197200
C	-3.63600700	-2.13882600	4.72719800
C	-4.95937200	-0.15549400	4.20176800
C	-2.30399900	-4.48104600	3.90891200
H	-2.92805000	-4.01768500	1.92848800
C	-2.94398900	-2.95747700	5.67389100
C	-4.28095700	-0.96292800	5.11926900
C	-2.30063200	-4.09890800	5.28056100
H	-1.75951300	-5.36842200	3.60032300
H	-2.93711700	-2.64578800	6.71570100
H	-4.25589600	-0.66873300	6.16679500
H	-1.77261600	-4.70994600	6.00738600
C	0.69198300	-4.32825700	-3.78107900
H	-0.03217600	-5.11673100	-3.96849600
C	0.28510400	-3.01977000	-3.78366800
H	-0.75387100	-2.78822400	-3.98656500
C	2.05000900	-4.67139700	-3.53027200
H	2.34776700	-5.71596900	-3.50717600
C	2.97418100	-3.68251400	-3.33349500
H	4.01707800	-3.92033900	-3.14430100
C	-6.37504900	1.43064000	2.35370000
H	-6.93271200	2.04401600	1.65085800
C	-6.29853000	1.82461000	3.71976700
H	-6.79274800	2.73533900	4.04708800
C	-5.61291400	1.04797600	4.61421600

H	-5.55516200	1.32933300	5.66322800
C	-5.76099200	0.28501500	1.91831100
H	-5.84288600	-0.00222400	0.87621100
C	1.17293600	2.02472200	3.22334000
H	1.32561900	0.94932100	3.09842900
H	2.09309100	2.56169700	2.98665900
H	0.95746000	2.18326600	4.29258600
C	-1.38770300	0.53654100	3.22254300
H	-0.54840800	-0.16071800	3.25897600
H	-1.60103300	0.86979100	4.24631600
H	-2.25492800	-0.02201400	2.87117600
C	-0.11426500	5.96784200	0.50832900
C	-1.02666900	6.69047400	1.29785600
C	0.76247100	6.71165500	-0.29481800
C	-1.04846700	8.08301500	1.30526000
H	-1.74694000	6.16278800	1.91685200
C	0.74149400	8.10964500	-0.29567500
H	1.48241700	6.21736500	-0.93646500
C	-0.15872100	8.80419400	0.50718900
H	-1.76489500	8.60446100	1.93479800
H	1.44100700	8.65046200	-0.92758700
H	-0.17049200	9.89064900	0.51154300
C	-1.53730200	3.94260000	-0.03688000
H	-1.46433900	2.87823100	-0.28605200
H	-2.26707500	4.02319700	0.77552200
C	-2.12649100	4.67772000	-1.23342200
C	-3.26940700	5.36576100	-1.07729900
H	-3.70245500	5.39292600	-0.07628300
C	-1.41923500	4.53248100	-2.55910700
H	-0.47667300	5.09510200	-2.57759400
H	-1.17594700	3.48055400	-2.75495900
H	-2.02207600	4.89140100	-3.39642600
C	-4.05385900	6.13827600	-2.09984300
H	-4.08900500	7.20345300	-1.83238300
H	-3.64251100	6.06835600	-3.11003800
H	-5.09578500	5.79179000	-2.13620300

TS-1-2-6RR

l imaginary frequency

H = -5393.912117

G = -5394.119156

E(M06-2X-DCM) = -5394.844611

0	1.47345600	-0.90580900	1.87484900
0	3.24808300	-0.20082000	0.09463000

P	1.66686500	-0.49118700	0.31727200
O	0.96548800	0.84623000	0.01256000
N	1.27350900	-1.77239400	-0.55265700
S	-0.25179200	-2.17010700	-0.80747400
C	-0.31496100	-3.92910100	-0.18223700
F	0.06386200	-3.97720400	1.09480500
F	0.49424400	-4.71168000	-0.90672400
F	-1.56787000	-4.37725200	-0.29122400
C	-0.49370800	4.37790700	-1.25354000
C	-0.58730400	3.66720700	-2.64639200
H	0.02637200	4.23960400	-3.35748700
H	-1.62473900	3.76144600	-2.97871800
C	-0.16734300	2.22250900	-2.81107600
C	-1.52070500	3.70508000	-0.29179700
H	-1.22513400	3.83750200	0.74830700
H	-2.47222700	4.22016900	-0.40841300
N	-1.81201500	2.28949300	-0.51672900
C	-3.06696700	1.84580400	-0.87717000
N	-3.20638700	0.49180200	-0.75398500
C	-4.33880800	-0.33747300	-0.92450000
C	-5.38448500	-0.09436200	-1.82647000
C	-4.36693400	-1.50748800	-0.15118800
C	-6.44567400	-0.99651000	-1.91227200
C	-5.43628800	-2.39452100	-0.25044600
H	-3.54561100	-1.72435400	0.52122000
C	-6.49239000	-2.14685800	-1.12490200
H	-7.32767000	-2.83249200	-1.19475300
C	-5.45664800	-3.59143500	0.66016900
C	-7.52968600	-0.75851700	-2.93150800
F	-5.78247400	-3.23734500	1.93739900
F	-6.35696000	-4.51782700	0.27426900
F	-4.25081500	-4.19400600	0.73173000
F	-8.71559000	-1.27021000	-2.52895000
F	-7.71650100	0.55437400	-3.17877300
F	-7.23442100	-1.34458200	-4.11638300
S	-4.26446300	2.88880400	-1.45837900
C	-1.01777800	5.84795300	-1.50427300
H	-1.95628000	5.75197900	-2.06145800
H	-0.30814500	6.35637500	-2.16982400
H	-5.37714000	0.79408600	-2.43948100
C	1.10241400	1.75111300	-2.48600900
H	-2.40728700	-0.02807500	-0.38156400
H	1.83500200	2.52137800	-2.24213100
O	-1.20312700	-1.44144000	0.07347700

H	-1.20514200	1.62737300	-0.03779100
O	-0.57984700	-2.24240300	-2.23599200
H	0.93355300	1.30582100	-1.20821700
C	5.98898100	-3.26051400	0.96169000
C	5.46311700	-2.47135100	1.97724100
C	4.60761200	-1.39559300	1.68556500
C	4.79337600	-1.91199400	-0.69403900
C	5.67971100	-2.94986600	-0.36043500
C	1.75760900	-0.05122800	2.94611000
C	3.08751800	0.19435200	3.27691100
C	3.38580400	1.19519300	4.21456800
C	2.36506800	1.81212200	4.93170300
C	1.04754500	1.40369000	4.72021600
C	0.70127600	0.47930400	3.71686200
H	6.12476400	-3.52059800	-1.16991000
H	0.25460300	1.81075300	5.33963700
C	4.35969200	-0.58055900	2.95164000
C	4.57383100	-1.69155500	4.03964100
H	3.64533300	-2.26543100	4.13960300
H	4.81315300	-1.27292500	5.02147700
H	5.26805500	1.03614100	5.28317100
H	5.17089900	2.45041000	4.24346600
C	4.21344600	-1.18590400	0.36449500
H	6.64875400	-4.09381100	1.18912300
H	2.58751300	2.56765200	5.68102700
C	5.68159500	-2.59627100	3.46751900
H	5.60649400	-3.63173200	3.81826900
H	6.68067300	-2.23826000	3.75339300
C	4.88413700	1.39502600	4.31856800
C	5.42567600	0.54790700	3.14297700
H	5.46526100	1.15421100	2.23053900
H	6.42872000	0.14928100	3.32313500
C	-0.71527300	0.02663700	3.56194600
C	-1.75410500	0.96516200	3.32803800
C	-1.02975800	-1.34825000	3.73523900
C	-1.53264100	2.37711000	3.21189200
C	-3.12009700	0.50261900	3.20889100
C	-2.39270600	-1.79722600	3.56644800
C	-2.57239100	3.25658700	3.04302400
H	-0.51973500	2.75766300	3.27558500
C	-4.17052100	1.45068500	3.00194500
C	-3.39766700	-0.86354000	3.30148400
C	-3.91289600	2.79258300	2.93228000
H	-2.37050900	4.32259200	2.97776300

H	-5.18643000	1.07602500	2.90592700
H	-4.42077700	-1.20940600	3.17445500
H	-4.72040600	3.50214800	2.77930900
C	4.62334500	-1.58789500	-2.14655500
C	3.95048100	-2.48658700	-3.00788800
C	5.28361900	-0.44883100	-2.67442500
C	3.25371000	-3.64261400	-2.53020700
C	3.94697900	-2.24074600	-4.43301500
C	5.25785000	-0.20817100	-4.10000700
C	2.62240600	-4.49836700	-3.39401100
H	3.20232500	-3.81834300	-1.46286800
C	3.28113500	-3.16332800	-5.29945800
C	4.59681900	-1.11126800	-4.93742200
C	2.64140700	-4.26386300	-4.79831600
H	2.08314000	-5.35575800	-3.00311500
H	3.29350600	-2.96568700	-6.36877700
H	4.59352200	-0.93324500	-6.01113700
H	2.13463000	-4.95571500	-5.46542900
C	-0.40267400	-3.65168100	4.26828000
H	0.35519200	-4.37139800	4.56634000
C	-0.06311100	-2.33278100	4.11781200
H	0.95665600	-2.02267700	4.31285800
C	-1.73485400	-4.09415000	4.03636900
H	-1.97971600	-5.14764300	4.13876400
C	-2.70232900	-3.18775600	3.69977800
H	-3.72627000	-3.50387800	3.52447400
C	6.63921500	1.56940400	-2.40712500
H	7.18306800	2.25628100	-1.76398500
C	6.59462900	1.81018700	-3.80953900
H	7.09951500	2.67848800	-4.22422000
C	5.92463900	0.94155600	-4.62788000
H	5.89017300	1.10622000	-5.70241400
C	6.01023200	0.48061600	-1.86159000
H	6.06550900	0.31111600	-0.79226200
C	0.95754700	4.42992900	-0.73588200
C	1.94129200	5.08279700	-1.50386300
C	1.36456400	3.87646000	0.48448800
C	3.26129000	5.18388300	-1.07105300
H	1.67801700	5.52241300	-2.46239600
C	2.68769900	3.97608600	0.92608200
H	0.66396800	3.33219500	1.10497700
C	3.64238100	4.63297500	0.15474700
H	3.99243400	5.69404300	-1.69274100
H	2.96269100	3.52404100	1.87524800

H	4.67098900	4.71066700	0.49614400
C	-1.27337900	6.72904000	-0.29027600
C	-2.54390700	6.98020100	0.07279700
H	-3.33387700	6.51457300	-0.51829600
C	-0.06731000	7.33015800	0.39525800
H	0.52576300	6.57323400	0.92086100
H	0.60551800	7.78830600	-0.34129200
H	-0.34165500	8.10133000	1.11891400
C	-1.13265700	1.33207700	-3.53392800
H	-1.06375200	0.28740700	-3.21662500
H	-2.16367300	1.67982300	-3.44783500
H	-0.86260300	1.34572900	-4.60247300
C	1.68566600	0.51844700	-3.17263500
H	1.02933900	-0.35347500	-3.13464700
H	1.89895400	0.73864000	-4.22632600
H	2.62701600	0.24149200	-2.69840000
C	-3.04882700	7.83287400	1.20285000
H	-3.66302700	7.23637700	1.89144700
H	-2.25253000	8.29888600	1.78875600
H	-3.70027200	8.63237900	0.82428300

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l imaginary frequency

H = -5393.909904

G = -5394.117556

E(M06-2X-DCM) = -5394.843341

O	1.37905900	-0.96764600	1.88623100
O	3.16878500	-0.42223400	0.06588100
P	1.57499000	-0.59938900	0.31714500
O	0.95948500	0.77459400	-0.00841600
N	1.08435300	-1.87100100	-0.51725700
S	-0.46793000	-2.17168600	-0.74026800
C	-0.63482200	-3.91141500	-0.08119100
F	-0.23735200	-3.96238900	1.19020300
F	0.10876200	-4.75816700	-0.80415700
F	-1.91595200	-4.27851500	-0.16098000
C	-0.22373000	4.38386400	-1.32829200
C	-0.36562800	3.66905100	-2.71478000
H	0.31633500	4.16389000	-3.42087200
H	-1.38165000	3.86776800	-3.06812000
C	-0.09536600	2.18632700	-2.85256700
C	-1.34030000	3.83236500	-0.39228100
H	-1.09413400	4.00942500	0.65510600
H	-2.25360600	4.38632200	-0.60427200

N	-1.70762700	2.42643500	-0.55611500
C	-2.99128400	2.03878300	-0.88374200
N	-3.19853700	0.69793000	-0.72617800
C	-4.37641300	-0.07029200	-0.88355300
C	-5.37864700	0.19019000	-1.82875200
C	-4.49706200	-1.19618100	-0.05721700
C	-6.49012900	-0.64953600	-1.90561100
C	-5.61448000	-2.02353700	-0.14990500
H	-3.70976300	-1.42774900	0.64991400
C	-6.62803600	-1.75606500	-1.06722800
H	-7.50072400	-2.39394800	-1.13149600
C	-5.72667600	-3.17772700	0.80786900
C	-7.52830500	-0.39792800	-2.96824300
F	-6.01797900	-2.74882000	2.07029400
F	-6.69814400	-4.04515500	0.45974800
F	-4.57146000	-3.87012600	0.90220300
F	-8.75408500	-0.81733100	-2.57888700
F	-7.62717800	0.90996100	-3.28353000
F	-7.23614000	-1.05843700	-4.11412200
S	-4.14761700	3.12568000	-1.46742800
C	-0.55366600	5.90432000	-1.61240300
H	-1.53436300	5.93139800	-2.10629100
H	0.17340800	6.26439200	-2.34736000
H	-5.29894500	1.04453400	-2.48374000
C	1.12786100	1.60178100	-2.53128900
H	-2.42851600	0.14199300	-0.34421100
H	1.93362800	2.30423100	-2.31310800
O	-1.35381000	-1.36620200	0.14163300
H	-1.13009400	1.75066300	-0.05992000
O	-0.82555300	-2.24848400	-2.16147100
H	0.94540800	1.20594600	-1.24192100
C	5.70391100	-3.65402200	0.93613800
C	5.25151400	-2.81571300	1.94761500
C	4.46840500	-1.68681700	1.65328000
C	4.57709100	-2.24875100	-0.72063000
C	5.39455700	-3.34122400	-0.38536000
C	1.74352500	-0.12057200	2.93832700
C	3.09294400	0.02998700	3.24593500
C	3.47911500	1.01768100	4.16536500
C	2.51873600	1.71648100	4.89052600
C	1.17126800	1.40482200	4.70371900
C	0.74198000	0.49780700	3.71699000
H	5.78451600	-3.95326600	-1.19304700
H	0.42063900	1.87644600	5.33003200

C	4.30037600	-0.83885300	2.91092500
C	4.45378400	-1.94731300	4.01181900
H	3.48905000	-2.45295800	4.13463900
H	4.73808800	-1.53336900	4.98358700
H	5.36369700	0.73584700	5.20436000
H	5.34951600	2.14127200	4.14827000
C	4.06736300	-1.46849100	0.33558900
H	6.30769900	-4.52814800	1.16581800
H	2.80860300	2.46154900	5.62719000
C	5.48583900	-2.93509200	3.43587600
H	5.34471200	-3.95786800	3.80311800
H	6.51209000	-2.64383800	3.70055900
C	4.98937800	1.11013900	4.24184000
C	5.44741400	0.21292300	3.06819400
H	5.51208700	0.80414900	2.14738600
H	6.42290500	-0.25381400	3.23548100
C	-0.70688900	0.15271300	3.58641600
C	-1.67420700	1.16462100	3.35208300
C	-1.12313100	-1.19126200	3.78431900
C	-1.34804600	2.55489700	3.22282900
C	-3.07263300	0.80613900	3.25275200
C	-2.51846200	-1.53704600	3.63884900
C	-2.32078900	3.50930200	3.06108600
H	-0.30936400	2.85900100	3.27779300
C	-4.05038500	1.82910300	3.04582900
C	-3.45230800	-0.53346100	3.36882500
C	-3.69355600	3.14746100	2.96453400
H	-2.03990700	4.55784500	3.00193700
H	-5.09259700	1.53160200	2.96279100
H	-4.50032400	-0.80191100	3.25882100
H	-4.44695800	3.91502900	2.81558500
C	4.40489500	-1.93689600	-2.17554700
C	3.66173400	-2.80440300	-3.01094700
C	5.12915000	-0.85230800	-2.73344300
C	2.89602800	-3.90210700	-2.50215200
C	3.65366500	-2.58450100	-4.44026300
C	5.09839600	-0.63606300	-4.16283200
C	2.19612700	-4.72880400	-3.34105900
H	2.84750500	-4.05414500	-1.43107800
C	2.91572300	-3.47626600	-5.28018400
C	4.36865000	-1.50935400	-4.97440400
C	2.21097300	-4.52199700	-4.74974700
H	1.60554000	-5.54010800	-2.92662900
H	2.92589400	-3.29934600	-6.35315100

H	4.36179500	-1.35096900	-6.05118000
H	1.64950800	-5.19025600	-5.39683000
C	-0.66652200	-3.52691000	4.34851300
H	0.03805500	-4.29781900	4.64922400
C	-0.22920300	-2.24060400	4.17125800
H	0.81385300	-2.00634400	4.34807000
C	-2.03176400	-3.86944000	4.14103300
H	-2.35514400	-4.89917200	4.26491000
C	-2.93165700	-2.89732100	3.80043500
H	-3.97896600	-3.13699200	3.64355000
C	6.61572200	1.07839800	-2.52209200
H	7.21178700	1.74009800	-1.89914600
C	6.56702500	1.29607600	-3.92816000
H	7.12128800	2.12196800	-4.36581700
C	5.83064500	0.45815600	-4.72109800
H	5.79170400	0.60515600	-5.79804100
C	5.92556700	0.04267800	-1.94791300
H	5.98466100	-0.11049700	-0.87636300
C	1.20944400	4.29862700	-0.76924400
C	2.28383900	4.77793400	-1.54371900
C	1.51324900	3.80249900	0.50296900
C	3.59364200	4.76131900	-1.07066600
H	2.10137400	5.17228400	-2.54019200
C	2.82547100	3.78414200	0.98606500
H	0.73512900	3.39463200	1.13593600
C	3.87208500	4.26509800	0.20524300
H	4.39673100	5.13556600	-1.70020800
H	3.01866400	3.37965000	1.97597600
H	4.89257300	4.25038100	0.57834100
C	-0.56333600	6.86917400	-0.43414000
C	0.52521200	7.61694600	-0.18671500
H	1.38613100	7.47782400	-0.84072600
C	-1.84759900	6.97745500	0.36001100
H	-2.71857400	6.97466700	-0.30707400
H	-1.98556000	6.13574900	1.05031800
H	-1.89037300	7.89298200	0.95501500
C	-1.14949200	1.37971400	-3.54840400
H	-1.17572800	0.33929200	-3.21159100
H	-2.14173600	1.82560500	-3.45849200
H	-0.89175400	1.34848900	-4.61966100
C	1.58078900	0.30666200	-3.20107700
H	0.84688000	-0.49918100	-3.13474900
H	1.79551700	0.48566700	-4.26225600
H	2.49984700	-0.04863200	-2.73571200

C	0.74040800	8.62897200	0.90261100
H	1.03242500	9.60038700	0.48085000
H	-0.13960100	8.78664500	1.53134800
H	1.56388400	8.31592000	1.55944800

TS-1-2-6RR-2

l imaginary frequency

H = -5393.909283

G = -5394.116484

E(M06-2X-DCM) = -5394.843272

O	-1.59801400	-1.57892300	-1.36491800
O	-3.22021200	-0.05169800	-0.00265200
P	-1.67302800	-0.52637600	-0.13016500
O	-0.88303800	0.75788600	-0.44803700
N	-1.30205200	-1.34187200	1.19242200
S	0.21152800	-1.72456700	1.53544400
C	0.11691300	-3.58073900	1.71915300
F	-0.35899100	-4.13183900	0.60201700
F	-0.68513800	-3.90758600	2.74091500
F	1.34255400	-4.05244000	1.95893200
C	0.55710100	4.44663100	-0.99953100
C	0.64901300	4.50427600	0.55916800
H	-0.05783400	5.26764000	0.91123500
H	1.64813000	4.87288100	0.80354200
C	0.37592200	3.26233800	1.37924000
C	1.67498900	3.50803800	-1.52565000
H	1.53051600	3.30194800	-2.59037500
H	2.62251600	4.03147400	-1.43505000
N	1.87554300	2.25444700	-0.80233000
C	3.11691100	1.85400400	-0.35551800
N	3.12917900	0.57996100	0.13763100
C	4.21292900	-0.16548500	0.66616100
C	5.21488300	0.38083000	1.48020800
C	4.22348800	-1.54012600	0.40321100
C	6.22293700	-0.44159700	1.98201100
C	5.23516800	-2.34912300	0.92009600
H	3.43125300	-1.97713800	-0.19142200
C	6.25078800	-1.80925600	1.70453900
H	7.04208900	-2.43664500	2.09557100
C	5.22385800	-3.81177900	0.57031600
C	7.25916900	0.14218000	2.90638400
F	5.52434000	-4.01201400	-0.74562800
F	6.12050500	-4.52110800	1.28489900
F	4.00920700	-4.36719300	0.76830400

F	8.44366300	-0.50255600	2.80017100
F	7.48385700	1.44932600	2.65867500
F	6.87922500	0.04703000	4.20319400
S	4.47076900	2.86829400	-0.37532600
C	0.84852900	5.89638700	-1.57358900
H	-0.00576700	6.52008600	-1.29534500
H	0.80558200	5.80415300	-2.66734000
H	5.21473300	1.43596100	1.70893600
C	-0.87430800	2.64805800	1.42715200
H	2.27782100	0.01807500	0.05540600
H	-1.68259200	3.20938100	0.95453300
O	1.13772300	-1.51989600	0.39199500
H	1.16820400	1.53255900	-0.92751500
O	0.63356400	-1.21784800	2.84570600
H	-0.78743200	1.70473800	0.45423000
C	-6.13381600	-2.98054200	0.74575400
C	-5.64882600	-2.77567000	-0.54000000
C	-4.73531400	-1.74286700	-0.81073300
C	-4.77116200	-1.11266200	1.54805900
C	-5.72048500	-2.12571700	1.76461900
C	-1.93764200	-1.27905700	-2.68787900
C	-3.28147900	-1.14140600	-3.02680900
C	-3.61990500	-0.66370000	-4.30285000
C	-2.63857400	-0.49509500	-5.27467900
C	-1.31857600	-0.82689100	-4.96604300
C	-0.92615800	-1.21022600	-3.67036200
H	-6.12826500	-2.23747300	2.76470700
H	-0.56023800	-0.78719900	-5.74171800
C	-4.54935300	-1.60877400	-2.31936800
C	-4.87443200	-3.07751900	-2.76728400
H	-3.97525200	-3.69004700	-2.63401900
H	-5.16480700	-3.13812800	-3.82013000
H	-5.57789400	-1.18614600	-5.08015300
H	-5.36629500	0.53899500	-4.81609800
C	-4.24116800	-0.98359900	0.24937000
H	-6.83974200	-3.78042900	0.95375800
H	-2.89593500	-0.15480700	-6.27461700
C	-5.97218300	-3.55147400	-1.79609000
H	-5.95734500	-4.63543600	-1.63586200
H	-6.97506100	-3.30184300	-2.17021700
C	-5.11543300	-0.44816800	-4.41068500
C	-5.59267600	-0.62954800	-2.95120600
H	-5.54369000	0.32776700	-2.41930200
H	-6.61805300	-1.00369200	-2.87397100

C	0.48807500	-1.61727700	-3.40509800
C	1.55932900	-0.72302300	-3.66314300
C	0.76082200	-2.94333000	-2.97473700
C	1.37488800	0.60447800	-4.17229700
C	2.92029500	-1.15111200	-3.42326700
C	2.12362600	-3.34247200	-2.70785400
C	2.44042100	1.42328000	-4.45010600
H	0.36870500	0.95806300	-4.36270200
C	4.00040200	-0.25463200	-3.69728300
C	3.16328300	-2.43593800	-2.93113500
C	3.77533700	0.99590300	-4.20457100
H	2.26446900	2.41406700	-4.86143100
H	5.01248800	-0.59555600	-3.49478700
H	4.18566100	-2.74164200	-2.72240500
H	4.60494500	1.66530500	-4.41049300
C	-4.47584500	-0.18918200	2.68928200
C	-3.80551400	-0.66984700	3.83988300
C	-5.01465500	1.12288400	2.67090900
C	-3.21309200	-1.97187300	3.90370100
C	-3.68956300	0.17903300	5.00479400
C	-4.87433200	1.96624100	3.83713700
C	-2.57757000	-2.40810200	5.03628200
H	-3.24022200	-2.60275500	3.02411600
C	-3.02761500	-0.32031000	6.17004600
C	-4.22540700	1.46910700	4.97103600
C	-2.49093900	-1.57859300	6.19030800
H	-2.11498900	-3.39036200	5.04811700
H	-2.95642800	0.32909800	7.03945400
H	-4.13783200	2.10259800	5.85172600
H	-1.98419900	-1.94515200	7.07877700
C	0.04907100	-5.21315200	-2.40699200
H	-0.74364900	-5.95048900	-2.31173400
C	-0.25210400	-3.94444500	-2.82763100
H	-1.27790400	-3.69712900	-3.07393100
C	1.38668400	-5.57926700	-2.08921600
H	1.60239300	-6.58395500	-1.73661800
C	2.39484500	-4.66753100	-2.24131400
H	3.42259800	-4.92825800	-2.00775500
C	-6.23588200	2.93288100	1.56864600
H	-6.77231500	3.31152600	0.70254700
C	-6.07811700	3.76455300	2.71337200
H	-6.48986600	4.77022300	2.71070500
C	-5.41870800	3.28855900	3.81417900
H	-5.29966300	3.90771300	4.70043100

C	-5.72654300	1.66046100	1.55003300
H	-5.86799600	1.04072300	0.67199100
C	-0.86412700	4.10720000	-1.49713100
C	-1.96233100	4.86562500	-1.04744800
C	-1.11984300	3.12365600	-2.45868900
C	-3.25012500	4.64837900	-1.53078000
H	-1.81669600	5.64585700	-0.30452600
C	-2.40882700	2.90291400	-2.95329000
H	-0.31891800	2.49510600	-2.82749400
C	-3.47983800	3.66415100	-2.49467700
H	-4.07314600	5.25000500	-1.15429200
H	-2.56679700	2.12380700	-3.69364800
H	-4.48244500	3.49415800	-2.87796000
C	2.12272200	6.63276800	-1.17882100
C	2.07823800	7.50758000	-0.15838400
H	1.12199000	7.63616300	0.35289400
C	3.36539200	6.40560200	-2.01714100
H	3.97058400	5.56502900	-1.65407200
H	3.09493400	6.18238500	-3.05610200
H	4.01347900	7.28655500	-2.03080200
C	1.46413000	2.82191700	2.30914500
H	1.43858200	1.74766600	2.51112200
H	2.45568300	3.11230000	1.95610800
H	1.29419100	3.32233200	3.27669500
C	-1.30062400	1.82153500	2.63818900
H	-0.59069100	1.03562300	2.90462700
H	-1.43363800	2.47236500	3.51154000
H	-2.25696800	1.33955600	2.43866400
C	3.19204600	8.35285000	0.39129300
H	3.38739800	8.10013400	1.44258900
H	4.13165400	8.23099700	-0.15289100
H	2.92206500	9.41763000	0.37284000

TS-1-2-6RR-3

l imaginary frequency

H = -5393.909016

G = -5394.115606

E(M06-2X-DCM) = -5394.843883

O	-1.62420300	-1.47539500	-1.45091600
O	-3.24626700	-0.01004700	-0.02289300
P	-1.70065700	-0.48731600	-0.16376700
O	-0.89998000	0.80533400	-0.40875400
N	-1.34540300	-1.37365100	1.11732000
S	0.16338600	-1.77803000	1.45472500

C	0.06193100	-3.64073500	1.54532500
F	-0.40389500	-4.13379700	0.39733100
F	-0.75123700	-4.01574400	2.54138000
F	1.28390400	-4.12743900	1.77363300
C	0.62298200	4.50296000	-0.72675200
C	0.70437900	4.46016200	0.83328300
H	0.02392300	5.22328000	1.23408100
H	1.71965500	4.76297100	1.10115300
C	0.38309200	3.17942000	1.57385500
C	1.73535700	3.57718700	-1.28721300
H	1.59857300	3.42529600	-2.36221900
H	2.68484800	4.09495500	-1.15842200
N	1.91355100	2.28740800	-0.62485300
C	3.14871800	1.84718300	-0.19293900
N	3.13923100	0.54695300	0.22860500
C	4.20902900	-0.24412400	0.71620800
C	5.22120600	0.24055100	1.55643200
C	4.19560300	-1.60309200	0.38057000
C	6.21532200	-0.62478100	2.01183400
C	5.19403500	-2.45554400	0.85130300
H	3.39544800	-1.99397200	-0.23534100
C	6.21966600	-1.97581600	1.66151000
H	7.00053900	-2.63664600	2.01675800
C	5.15990500	-3.89649500	0.42219400
C	7.26188400	-0.10896300	2.96449300
F	5.46884900	-4.03036100	-0.90031700
F	6.03765800	-4.65975600	1.10404800
F	3.93406500	-4.44016000	0.57974500
F	8.43432700	-0.76922600	2.82453500
F	7.51106000	1.20483200	2.78464700
F	6.87978300	-0.26387300	4.25495300
S	4.51254900	2.84373700	-0.14902200
C	0.96650100	5.96571000	-1.24114800
H	0.09100900	6.59534100	-1.04968500
H	1.03566200	5.88044300	-2.33295600
H	5.23929900	1.28194400	1.84047200
C	-0.88288700	2.59567300	1.56125900
H	2.28010000	0.00371700	0.11002500
H	-1.66612700	3.20307000	1.10397000
O	1.10190600	-1.52095100	0.33192300
H	1.20453200	1.57879100	-0.80416900
O	0.57497300	-1.33722900	2.79222100
H	-0.79781800	1.70369400	0.54561100
C	-6.18886600	-2.95320300	0.53037200

C	-5.69037100	-2.67886800	-0.73715600
C	-4.76604200	-1.64014700	-0.93988800
C	-4.82034400	-1.14484100	1.45041400
C	-5.77885000	-2.16129100	1.60018100
C	-1.94581600	-1.09847100	-2.75859400
C	-3.28432600	-0.92720400	-3.10301600
C	-3.60409300	-0.37310100	-4.35260100
C	-2.61036800	-0.15940600	-5.30280500
C	-1.29736800	-0.52326400	-5.00035200
C	-0.92294500	-0.98462200	-3.72486200
H	-6.19725900	-2.32640300	2.58843800
H	-0.53039900	-0.44751000	-5.76476900
C	-4.56390600	-1.42152500	-2.43650000
C	-4.89767600	-2.85904400	-2.97113600
H	-4.00517900	-3.48649900	-2.86524400
H	-5.17858200	-2.85637900	-4.02829400
H	-5.55849900	-0.82913900	-5.17919300
H	-5.33313100	0.87541400	-4.81262200
C	-4.27627600	-0.94658800	0.16630100
H	-6.90282700	-3.75788200	0.68584000
H	-2.85314100	0.24079700	-6.28403200
C	-6.00860800	-3.37798700	-2.03874500
H	-6.00483200	-4.46948300	-1.94131200
H	-7.00568100	-3.09778700	-2.40671800
C	-5.09624400	-0.13624400	-4.46303000
C	-5.59133000	-0.39747600	-3.02158700
H	-5.54015300	0.52693200	-2.43455100
H	-6.62077300	-0.76579400	-2.97727400
C	0.48375500	-1.42157000	-3.46772700
C	1.56740600	-0.52668400	-3.66457800
C	0.73738800	-2.77210700	-3.10734800
C	1.40310300	0.82868900	-4.10215700
C	2.92081000	-0.98249500	-3.43308900
C	2.09261000	-3.20044200	-2.84737300
C	2.48059400	1.64917300	-4.32322200
H	0.40311300	1.20388600	-4.28361300
C	4.01360600	-0.08475600	-3.64571200
C	3.14437200	-2.29481000	-3.00902300
C	3.80791400	1.19391000	-4.08676300
H	2.31990400	2.66286300	-4.68158800
H	5.01947400	-0.44761000	-3.45047300
H	4.16088100	-2.62292800	-2.80574000
H	4.64703500	1.86405300	-4.24661400
C	-4.53206600	-0.28778700	2.64418500

C	-3.87216700	-0.83323800	3.77155100
C	-5.06885000	1.02427900	2.69466500
C	-3.28454300	-2.13896600	3.76830700
C	-3.76343600	-0.05034500	4.98252500
C	-4.93612600	1.80139300	3.90690500
C	-2.65995200	-2.63927200	4.88030000
H	-3.30664900	-2.72038000	2.85510000
C	-3.11234800	-0.61535700	6.12365900
C	-4.29628400	1.24096600	5.01616700
C	-2.57990400	-1.87478700	6.07884600
H	-2.20099300	-3.62252300	4.84193800
H	-3.04633200	-0.01512100	7.02811000
H	-4.21431600	1.82446200	5.93127300
H	-2.08165600	-2.29159900	6.94979400
C	-0.00501600	-5.06128600	-2.67148600
H	-0.80661000	-5.79372700	-2.62526800
C	-0.28769200	-3.76839500	-3.02617800
H	-1.30780300	-3.49676200	-3.27041000
C	1.32481400	-5.45907500	-2.35925700
H	1.52575200	-6.48375500	-2.05939300
C	2.34431100	-4.55186200	-2.45073700
H	3.36645400	-4.83646700	-2.22064500
C	-6.27977300	2.89465600	1.68576000
H	-6.80909400	3.32184100	0.83806300
C	-6.12967800	3.66112700	2.87611300
H	-6.54032600	4.66599600	2.92633200
C	-5.47880600	3.12376500	3.95350400
H	-5.36557400	3.69250600	4.87365600
C	-5.77156500	1.62454700	1.60008600
H	-5.90681900	1.05492500	0.68778300
C	-0.79739800	4.21983800	-1.25675100
C	-1.88212400	4.98388000	-0.78416800
C	-1.06472400	3.28505100	-2.26217800
C	-3.16987100	4.81623000	-1.28651100
H	-1.72383800	5.72910700	-0.00825700
C	-2.35386900	3.11497200	-2.77659600
H	-0.27380200	2.65580600	-2.65091300
C	-3.41199800	3.87902600	-2.29370900
H	-3.98309900	5.41963300	-0.89197600
H	-2.52220400	2.37220600	-3.55127700
H	-4.41463200	3.74773200	-2.69180400
C	2.20177100	6.68019100	-0.71090300
C	3.37149000	6.57972600	-1.36500500
H	3.38712000	5.96156800	-2.26369600

C	1.98782500	7.56841900	0.49576700
H	1.22941500	8.33250100	0.27334800
H	1.61954000	7.01223200	1.36608500
H	2.89727600	8.08811300	0.80424300
C	1.43867300	2.65977000	2.50064200
H	1.38524700	1.57592300	2.63554300
H	2.44473200	2.94762200	2.18903700
H	1.25540400	3.10317800	3.49325300
C	-1.35612700	1.71852800	2.71844900
H	-0.67338200	0.89979500	2.95529500
H	-1.48872700	2.32567500	3.62278000
H	-2.32138000	1.27600700	2.47498400
C	4.70001400	7.19392300	-1.03068100
H	5.06598200	7.80764200	-1.86501000
H	4.67912800	7.82182700	-0.13650800
H	5.44622100	6.40510200	-0.86843000

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0 imaginary frequency

H = -5472.521040

G = -5472.736862

E(M06-2X-DCM) = -5473.496169

C	4.17567300	-2.43512400	0.92343500
C	4.68492900	-1.52559600	2.10644400
H	3.85686600	-0.87221100	2.38764800
H	4.85472100	-2.18574900	2.96772100
C	5.95170000	-0.70144900	1.92116200
C	4.13667200	-1.62673300	-0.39597300
H	3.97928900	-2.29714800	-1.24841900
H	5.10197700	-1.14274400	-0.54691800
N	3.12737200	-0.57266200	-0.40512200
C	3.20613500	0.54835100	-1.16502100
N	2.05127600	1.30624400	-1.09976200
C	1.81174500	2.61041400	-1.54990100
C	2.80321500	3.60332700	-1.62060100
C	0.48914100	2.95352700	-1.86934000
C	2.46694700	4.89300200	-2.02429200
C	0.17292700	4.25136900	-2.26980100
H	-0.29146100	2.20382600	-1.79711500
C	1.15678100	5.23337400	-2.36311700
H	0.91140600	6.23658100	-2.68971500
C	-1.26020100	4.61662900	-2.52736500
C	3.51679700	5.97208700	-1.99731400
F	-1.38349600	5.64981900	-3.38474200

F	-1.89591800	4.98980000	-1.37902700
F	-1.97133100	3.58149300	-3.03355800
F	4.76071100	5.48635600	-2.16839800
F	3.51148300	6.63101700	-0.80685100
F	3.30406300	6.90491400	-2.95198600
S	4.55606900	0.93926800	-2.10198900
H	3.82527800	3.36326800	-1.36751700
C	5.94892100	0.64569000	1.80898600
H	1.22020600	0.81534000	-0.76583600
H	2.22367700	-0.80435900	-0.00174800
H	-0.79620400	-1.81606000	1.96982700
O	-1.81048100	1.19933400	0.69759600
O	-2.82290600	-0.87316000	-0.46284100
P	-1.53559000	-0.34677700	0.34918200
O	-0.18684200	-0.46637900	-0.25454000
C	-4.98736200	2.22260000	3.21985600
C	-5.23068200	1.88494700	1.89356300
C	-4.16723000	1.66338200	1.00329100
C	-2.58250200	2.01106000	2.83782800
C	-3.66966000	2.32924900	3.66686300
C	-3.23176900	-0.24785500	-1.66240200
C	-4.02436700	0.89476900	-1.59359200
C	-4.34524100	1.55400700	-2.79323800
C	-3.95555300	1.03554600	-4.02263100
C	-3.22764400	-0.15258600	-4.06178000
C	-2.83603300	-0.81510800	-2.88818500
H	-3.46651200	2.63248700	4.68951600
H	-2.92984400	-0.57783400	-5.01556600
C	-4.71270900	1.59241300	-0.42122100
C	-6.13413400	1.00587100	-0.13492000
H	-6.83477200	1.19022900	-0.95522500
H	-6.04815500	-0.07813100	0.00235700
H	-4.72290400	3.66913500	-3.11932300
H	-6.16580900	2.72551400	-2.74431600
C	-2.87577200	1.63058000	1.51509500
H	-5.81071600	2.40761500	3.90488700
H	-4.20886900	1.55120900	-4.94509200
C	-6.55720400	1.66899900	1.19624300
H	-7.08433000	2.61728800	1.02410000
H	-7.23092700	1.03589100	1.78412200
C	-5.09637900	2.83507400	-2.51664800
C	-4.85306700	3.04045300	-1.00898900
H	-5.64288500	3.61245700	-0.51403900
H	-3.91086300	3.57719600	-0.86469800

C	-2.05240300	-2.08794900	-2.99118300
C	-2.71280600	-3.32715100	-2.81205500
C	-0.68302400	-2.05026700	-3.34489400
C	-4.11402300	-3.42706100	-2.53579900
C	-1.96562300	-4.55768900	-2.93976100
C	0.05076100	-3.28939400	-3.47859700
C	-4.72472400	-4.64356500	-2.37386900
H	-4.69893300	-2.51698700	-2.46057900
C	-2.63848300	-5.80547600	-2.75139200
C	-0.60574000	-4.50430100	-3.26181700
C	-3.97833300	-5.85203900	-2.47464600
H	-5.79114500	-4.68951300	-2.16975900
H	-2.05901800	-6.72111400	-2.84343000
H	-0.04835600	-5.43348100	-3.36393800
H	-4.47880400	-6.80697400	-2.33990400
C	-1.17949300	2.11231900	3.34975900
C	-0.31640500	3.11008500	2.82893500
C	-0.73273200	1.25134600	4.38290600
C	-0.72000800	4.04347300	1.82138300
C	1.03298500	3.22153800	3.33547200
C	0.61590300	1.38513400	4.88868600
C	0.14595600	4.98585500	1.33156800
H	-1.73339100	4.00447900	1.43886900
C	1.90735900	4.21383300	2.79038200
C	1.45994500	2.35871700	4.34875500
C	1.48435700	5.06897100	1.80906400
H	-0.19223800	5.66979400	0.56001800
H	2.92310000	4.26890100	3.17437800
H	2.47570600	2.44926400	4.72823600
H	2.16285600	5.80022200	1.37989900
C	1.35158900	-0.82914300	-3.93249800
H	1.87228900	0.10859600	-4.10096100
C	0.02611900	-0.82898600	-3.58523000
H	-0.50544800	0.11149600	-3.49244900
C	2.07028800	-2.05285600	-4.05831300
H	3.12196000	-2.02628500	-4.32840400
C	1.43554300	-3.24560500	-3.83700500
H	1.97080000	-4.18733700	-3.93608200
C	-1.08399600	-0.59781800	5.94486100
H	-1.72783700	-1.37608600	6.34402800
C	0.24021100	-0.45208500	6.44701500
H	0.59249500	-1.10948700	7.23729400
C	1.06283600	0.51158100	5.92930500
H	2.07825600	0.63285200	6.29946900

C	-1.55273200	0.22377700	4.95260500
H	-2.56351900	0.09408800	4.58443800
N	-1.67040400	-1.35080500	1.71249800
S	-2.99299900	-2.08943600	2.45841300
C	-3.62915400	-3.37796200	1.22121500
O	-4.07610000	-1.13233300	2.61837700
O	-2.43089100	-2.85591500	3.56298600
F	-4.09636000	-4.40339500	1.93179700
F	-4.61062500	-2.86092300	0.49247200
F	-2.63771500	-3.79677200	0.43605600
C	2.78427500	-3.00815500	1.27125000
C	2.35351300	-3.17280600	2.59948700
C	1.90603900	-3.43338500	0.25678700
C	1.11878200	-3.75175600	2.90236300
H	2.98075500	-2.85239000	3.42276600
C	0.67331300	-4.01592600	0.55230100
H	2.18192700	-3.32111200	-0.78590700
C	0.27479100	-4.18797900	1.87945400
H	0.81747100	-3.86184400	3.94051600
H	0.02485900	-4.33036500	-0.26042900
H	-0.67826600	-4.65025500	2.11682700
C	5.19906800	-3.62159100	0.71534200
H	6.14366700	-3.17402000	0.40355300
H	5.38064800	-4.05246300	1.70853700
C	4.83420400	-4.76400500	-0.22186100
C	5.26447200	-4.84565900	-1.50040500
C	7.21385300	1.45724700	1.62582800
H	7.12578500	2.07893400	0.72486000
H	7.36155000	2.14922500	2.46790600
H	8.11810000	0.85663000	1.51934500
C	4.94783900	-6.02772500	-2.39108500
H	5.86705800	-6.57377700	-2.64897700
H	4.25334700	-6.74123800	-1.94463800
H	4.51796900	-5.68987400	-3.34500900
C	4.04600800	-5.90129000	0.41950800
H	4.65935900	-6.80868700	0.50545000
H	3.71816100	-5.63486300	1.42683400
H	3.14596300	-6.16919200	-0.14349300
C	7.26422300	-1.47544500	1.98322500
H	7.11965300	-2.45318600	2.45225800
H	7.70381800	-1.65798700	0.99304400
H	8.02118800	-0.94966300	2.57316900
C	4.72850000	1.53517900	1.85589900
H	3.78781000	1.01536800	2.03734200

H	4.85299700	2.29050800	2.64564100
H	4.62422300	2.08724300	0.91360400
C	6.12736000	-3.82061100	-2.20232500
H	6.48837100	-3.01830400	-1.55757600
H	7.00388800	-4.30916600	-2.65055100
H	5.58229500	-3.34786000	-3.03153000

INT-16'

0 imaginary frequency

H = -5472.493650

G = -5472.711885

E(M06-2X-DCM) = -5473.483783

O	-0.74907300	-2.68967600	-0.87803900
O	-2.71121700	-1.10400000	-0.24307000
P	-1.08111400	-1.25516300	-0.13938100
O	-0.44503500	-0.10126200	-0.85479000
C	-1.61451400	-2.94473200	-4.96851000
C	-2.60701100	-3.14545500	-4.01437800
C	-2.28889700	-3.14477600	-2.64936400
C	0.04142900	-2.66956200	-3.18033000
C	-0.30077100	-2.75015400	-4.54323900
C	-3.54349900	-2.08067000	0.31302900
C	-3.76697700	-3.26810800	-0.38982800
C	-4.46104400	-4.31826700	0.23291300
C	-5.01698900	-4.15590000	1.49576000
C	-4.90073700	-2.91813600	2.12359300
C	-4.17078300	-1.85910100	1.55771400
H	0.49153600	-2.64221200	-5.27803400
H	-5.37453900	-2.75339400	3.08687400
C	-3.47666100	-3.64533500	-1.84072700
C	-4.65162200	-3.22288600	-2.78567800
H	-4.88220700	-2.16677400	-2.60409000
H	-5.56335100	-3.80092800	-2.60534300
H	-5.47906200	-5.69776400	-1.09386600
H	-4.24650000	-6.46362900	-0.09705100
C	-0.99662000	-2.82372800	-2.24025900
H	-1.84800400	-2.96153400	-6.03035800
H	-5.55152400	-4.96941300	1.97972700
C	-4.08669700	-3.39604900	-4.21357600
H	-4.53800400	-2.70368500	-4.93427700
H	-4.27073300	-4.40925700	-4.59750600
C	-4.48531400	-5.54705200	-0.64861600
C	-3.43293900	-5.20664300	-1.72229600
H	-2.43782100	-5.50245300	-1.37080200

H	-3.60944800	-5.70351200	-2.68143200
C	-4.20992600	-0.54581800	2.28095700
C	-3.53436200	-0.38347700	3.51374800
C	-5.08097500	0.46814900	1.80934500
C	-2.66100500	-1.38180000	4.05076300
C	-3.72198400	0.82927700	4.27911400
C	-5.25038300	1.68108500	2.57848600
C	-2.02498200	-1.19908500	5.24979800
H	-2.47609600	-2.27770000	3.47336000
C	-3.04327100	0.97717200	5.52909800
C	-4.56733300	1.82821500	3.78930600
C	-2.22059400	-0.00778100	6.00428000
H	-1.34255900	-1.96036400	5.61486900
H	-3.19670400	1.89479700	6.09251600
H	-4.70739300	2.73771100	4.37064700
H	-1.70501700	0.11826800	6.95260100
C	1.48017700	-2.49183400	-2.81389600
C	2.18679800	-1.35235100	-3.27454300
C	2.17167200	-3.51865800	-2.12120700
C	1.54168900	-0.25165700	-3.92731900
C	3.61747500	-1.26932600	-3.08751500
C	3.59232300	-3.39022300	-1.88697500
C	2.25726300	0.81288900	-4.41373900
H	0.46222200	-0.26362500	-4.01537300
C	4.32967000	-0.14836900	-3.62366400
C	4.27931800	-2.28153100	-2.38808400
C	3.67424100	0.86234800	-4.27603000
H	1.74059900	1.62637900	-4.91804400
H	5.40939700	-0.11957100	-3.49799700
H	5.35105700	-2.20145900	-2.22339300
H	4.22936100	1.70193800	-4.68644300
C	-6.71173800	1.32133100	0.19603100
H	-7.30093400	1.18153500	-0.70697200
C	-5.85732300	0.33260500	0.61305500
H	-5.77229800	-0.58235100	0.03759400
C	-6.84749300	2.52827300	0.94020500
H	-7.52555300	3.30325000	0.59266500
C	-6.13606900	2.69652300	2.09760200
H	-6.24115100	3.60557700	2.68570500
C	2.23200600	-5.68037200	-0.98178800
H	1.71779400	-6.57309000	-0.63636200
C	3.62388000	-5.53119000	-0.72509600
H	4.15801900	-6.30543900	-0.18117300
C	4.28230200	-4.41911300	-1.17309800

H	5.34843300	-4.29590400	-0.99826300
C	1.53520600	-4.71465700	-1.65908200
H	0.47883900	-4.85619200	-1.85108000
C	-1.17283600	3.92476600	-1.57188000
C	-1.58057300	4.32425600	-0.10789400
H	-1.34866400	5.38490800	-0.02283200
H	-2.67190800	4.26342100	-0.02701000
C	-0.97338800	3.57956900	1.07449700
C	0.35767500	3.69314400	-1.63203900
H	0.80679800	4.49958600	-1.05194100
H	0.71655700	3.77785500	-2.66394500
N	0.83605400	2.41386900	-1.08222000
C	2.04540700	2.20661900	-0.58462800
N	2.38757300	1.03972900	-0.03331300
C	3.64742000	0.79190400	0.61375300
C	4.80852400	0.64812300	-0.14315200
C	3.67889800	0.65743100	2.00421200
C	6.02137700	0.39770600	0.50291400
C	4.89533200	0.39485400	2.63289200
H	2.76212700	0.72419000	2.57980900
C	6.07047300	0.27083100	1.88960800
H	7.01177000	0.07328800	2.38767600
C	4.92608700	0.19420300	4.12827800
C	7.28114900	0.31096700	-0.31692600
F	6.15362900	0.45615700	4.63553600
F	4.61928300	-1.07367900	4.46526300
F	4.04676400	1.00282200	4.75318200
F	8.29038700	-0.27127100	0.35909000
F	7.70778800	1.53494100	-0.70270900
F	7.09017500	-0.40444200	-1.45539800
S	3.32972200	3.44151400	-0.57593400
H	4.75893800	0.72322400	-1.22291100
H	1.69650800	0.27731100	0.03046300
H	0.20101600	1.59367200	-1.07503600
C	-0.03567300	4.12845700	1.88171300
H	2.69305500	4.32157600	-1.36625000
N	-0.79269700	-1.51432200	1.42725400
S	0.66931400	-1.57127700	2.02863000
O	0.82397200	-0.72738900	3.22468800
O	1.74826800	-1.48063000	1.00986300
C	0.78867500	-3.32308500	2.66460600
F	-0.14681600	-3.54730500	3.60149300
F	1.99358000	-3.51861600	3.21075100
F	0.61449200	-4.19451500	1.66779500

C	-1.95966200	2.76512300	-2.21733900
C	-3.25185600	2.40851900	-1.80758400
C	-1.45072900	2.13005000	-3.36426000
C	-3.99768000	1.45861800	-2.50745600
H	-3.70036500	2.85797000	-0.92923600
C	-2.19106100	1.18000000	-4.06542300
H	-0.45694100	2.37271300	-3.72868700
C	-3.47466400	0.84079400	-3.64071500
H	-4.98911900	1.20311300	-2.14770300
H	-1.76239000	0.70476600	-4.94374300
H	-4.05606000	0.10198000	-4.18529000
C	-1.50157500	5.16873500	-2.51156000
H	-1.26610400	4.85961000	-3.53785400
H	-2.58889400	5.26821300	-2.48116100
C	-0.83540900	6.51182000	-2.25058800
C	-1.44671000	7.53598500	-1.61227500
C	-1.60991000	2.23298200	1.33399400
H	-1.04288100	1.58571700	2.00331100
H	-2.60258000	2.37263900	1.78208500
H	-1.76708700	1.67936700	0.40601700
C	0.56240300	6.67964200	-2.83818000
H	0.76533700	5.91035200	-3.59009300
H	0.68740400	7.64555700	-3.33698200
H	1.35766300	6.61261500	-2.08129800
C	0.51923600	3.44242500	3.11376300
H	0.20720400	2.40496300	3.23523400
H	1.61843200	3.46365200	3.10482100
H	0.21533300	3.98576700	4.02061500
C	-0.78092500	8.87639900	-1.38250600
H	0.28211700	8.89233300	-1.62795500
H	-1.27623200	9.66206100	-1.97130600
H	-0.88079800	9.17405700	-0.33015700
C	-2.85460100	7.50382100	-1.06040500
H	-3.41780600	6.60551100	-1.31589500
H	-2.84413600	7.58477000	0.03536100
H	-3.42041000	8.37109000	-1.42765800
C	0.56112400	5.51309300	1.71590100
H	0.21582000	6.06224400	0.83743400
H	0.33637300	6.13064100	2.59782400
H	1.65756300	5.45470900	1.66318500

INT-16' -1

0 imaginary frequency

H = -5472.493581

G = -5472.710711

E(M06-2X-DCM) = -5473.474167

O	-1.56074900	-2.27825500	-1.06511400
O	-3.21093700	-0.48782400	-0.15241500
P	-1.62096000	-0.88249300	-0.19430400
O	-0.87200900	0.22196800	-0.87658900
C	-3.03314500	-2.26081500	-4.98775500
C	-3.88605300	-2.43761900	-3.90329400
C	-3.37395200	-2.50767900	-2.60029900
C	-1.12082400	-2.14576100	-3.45783300
C	-1.66321400	-2.14887200	-4.75658900
C	-4.10174700	-1.35604600	0.49497300
C	-4.52501900	-2.51611000	-0.15754200
C	-5.23656400	-3.48916400	0.56290500
C	-5.62356200	-3.25919000	1.87759400
C	-5.32596100	-2.02769500	2.45849900
C	-4.56478400	-1.05340600	1.79169500
H	-0.98332600	-2.04483400	-5.59698800
H	-5.67525100	-1.80368200	3.46218900
C	-4.46937900	-2.92126700	-1.62864800
C	-5.73136900	-2.39520000	-2.39567200
H	-5.85503500	-1.32838000	-2.17604900
H	-6.64927700	-2.90659900	-2.09017900
H	-6.52745800	-4.78982200	-0.59835400
H	-5.24351100	-5.64718900	0.24701700
C	-2.01479100	-2.29702200	-2.37903800
H	-3.42066700	-2.22077200	-6.00267000
H	-6.17100500	-4.01246000	2.43854100
C	-5.39192400	-2.58207700	-3.89038200
H	-5.89117900	-1.84807700	-4.53339900
H	-5.69770800	-3.57463400	-4.25009800
C	-5.47581700	-4.71848400	-0.28673300
C	-4.54513200	-4.47836300	-1.49402100
H	-3.54211600	-4.85887800	-1.26921000
H	-4.88915200	-4.96159800	-2.41408300
C	-4.40698200	0.27944100	2.46123000
C	-3.57114300	0.43079500	3.59217500
C	-5.25434400	1.34124400	2.05464300
C	-2.73153300	-0.62119400	4.07870700
C	-3.55758400	1.68834100	4.30749000
C	-5.25075600	2.58209400	2.79608900
C	-1.93428200	-0.44324800	5.17833200
H	-2.70912900	-1.56103400	3.54301600
C	-2.70799500	1.83277600	5.44880000

C	-4.39311300	2.72674300	3.88967900
C	-1.91986600	0.79834400	5.87524700
H	-1.28560600	-1.25002100	5.50461500
H	-2.70849700	2.78586900	5.97296600
H	-4.39329300	3.66354800	4.44379800
H	-1.27758300	0.91966900	6.74362900
C	0.36236600	-2.02768500	-3.30815600
C	1.02671400	-0.88045200	-3.81139800
C	1.11694200	-3.10672900	-2.78067800
C	0.32659700	0.26432800	-4.31757400
C	2.47197300	-0.83734200	-3.82915500
C	2.56060000	-3.02975000	-2.76513000
C	0.99378200	1.33269300	-4.86011800
H	-0.75538300	0.27727000	-4.26291100
C	3.13177900	0.29454300	-4.40697300
C	3.19867600	-1.90654700	-3.30024900
C	2.41802200	1.34453400	-4.92279600
H	0.43466200	2.18059600	-5.24655600
H	4.21900800	0.28734200	-4.44802100
H	4.28628500	-1.87058700	-3.31485400
H	2.93040300	2.18144200	-5.39091000
C	-7.02652300	2.25222000	0.63272400
H	-7.72020900	2.13195000	-0.19545600
C	-6.17369700	1.22982800	0.96106700
H	-6.20367300	0.30538000	0.39540700
C	-7.02388200	3.46854400	1.37375800
H	-7.71479400	4.26440800	1.10781400
C	-6.15417800	3.62489700	2.41992700
H	-6.14163800	4.54664800	2.99746300
C	1.27369100	-5.32048400	-1.75689000
H	0.78671800	-6.21080700	-1.36916900
C	2.69235600	-5.22229000	-1.71119500
H	3.27696400	-6.02898600	-1.27859900
C	3.31585100	-4.11298400	-2.21522000
H	4.39906300	-4.02860400	-2.19094000
C	0.51636000	-4.30496300	-2.27885100
H	-0.56141400	-4.40457900	-2.30864100
C	0.64115500	4.26496200	-0.74545100
C	1.43639000	4.41692600	0.60025800
H	2.48008800	4.56136700	0.30867800
H	1.12449800	5.38361600	1.02158400
C	1.38517900	3.37639900	1.72769400
C	1.19092200	3.09622000	-1.62210300
H	2.12553400	3.43936600	-2.05437600

H	0. 52397500	2. 89832000	-2. 46117300
N	1. 45233900	1. 80188900	-0. 96969300
C	2. 63144100	1. 32351400	-0. 60987600
N	2. 73294600	0. 18871400	0. 08675500
C	3. 92114600	-0. 33066800	0. 67792000
C	4. 69587900	0. 47260300	1. 51434600
C	4. 25765500	-1. 67166900	0. 47718400
C	5. 84338200	-0. 05056400	2. 10994400
C	5. 40502600	-2. 18239200	1. 08479700
H	3. 62234500	-2. 30350800	-0. 13198700
C	6. 20825700	-1. 37781800	1. 89528000
H	7. 09617300	-1. 78438800	2. 36269600
C	5. 80112600	-3. 61114900	0. 80713900
C	6. 63437700	0. 82887500	3. 04282200
F	6. 32371700	-3. 73853000	-0. 44047500
F	4. 74672300	-4. 44633400	0. 87446100
F	6. 73578800	-4. 05496000	1. 67197700
F	5. 99284900	1. 00503600	4. 22078600
F	6. 82028100	2. 06265600	2. 51512900
F	7. 84927400	0. 31587900	3. 31806000
S	4. 16770200	2. 13023300	-1. 08074800
H	4. 38154200	1. 48751100	1. 72733500
H	1. 89580900	-0. 40438100	0. 25706300
H	0. 62241900	1. 19632200	-0. 80639700
C	2. 41998600	3. 25992000	2. 59578700
H	3. 77827700	2. 30063400	-2. 36284600
N	-1. 25899500	-1. 31515600	1. 31759500
S	0. 13246700	-1. 88218400	1. 78788800
O	0. 56025300	-1. 34685400	3. 08460000
O	1. 16458600	-1. 92120700	0. 70661800
C	-0. 21471400	-3. 68826000	2. 11459400
F	0. 90348100	-4. 29474700	2. 52722700
F	-0. 65513300	-4. 29548800	1. 00834600
F	-1. 14568200	-3. 80358800	3. 07172200
C	-0. 88413800	4. 24412800	-0. 53745800
C	-1. 49015900	5. 28802300	0. 18514100
C	-1. 72408500	3. 26206000	-1. 07620800
C	-2. 87202600	5. 35613100	0. 34563400
H	-0. 87943200	6. 06802300	0. 63170200
C	-3. 11000100	3. 31995800	-0. 90658500
H	-1. 32251400	2. 40640400	-1. 60348500
C	-3. 69383800	4. 37177800	-0. 20612100
H	-3. 30631700	6. 17865700	0. 90860000
H	-3. 72658900	2. 52189800	-1. 30930400

H	-4.76906500	4.41145600	-0.06894600
C	1.01868300	5.57697100	-1.56413000
H	0.56422900	6.42044200	-1.03189100
H	2.09872900	5.70672500	-1.46199800
C	0.61729600	5.66843600	-3.02984200
C	1.50931100	5.57792300	-4.04367900
C	0.08621500	2.63318500	1.94839600
H	-0.71400900	3.33938900	2.20545100
H	-0.26697400	2.10442900	1.05940400
H	0.14652100	1.90558900	2.75760800
C	-0.85693700	5.94549900	-3.27371100
H	-1.03847300	6.45854500	-4.22053500
H	-1.46030500	5.02984600	-3.26494800
H	-1.26151700	6.57699700	-2.47618100
C	2.41045300	2.30526600	3.78051100
H	1.94665500	2.77033200	4.66249400
H	1.87985900	1.36915800	3.58940200
H	3.43565400	2.04576600	4.07066800
C	1.12499400	5.66997000	-5.50680300
H	0.05088800	5.62410100	-5.68918700
H	1.50565600	6.59962000	-5.95471300
H	1.58797600	4.84919900	-6.07232400
C	3.65331600	4.14431900	2.59538000
H	3.69885600	4.86967200	1.78172600
H	3.68718900	4.71403300	3.53584400
H	4.58220500	3.55802000	2.57504400
C	3.00405900	5.38915300	-3.88557000
H	3.31723500	4.40760500	-4.27210500
H	3.54198200	6.13453600	-4.48755000
H	3.36986800	5.47492800	-2.86074900

INT-16⁷-10

0 imaginary frequency

H = -5472.493185

G = -5472.711645

E(M06-2X-DCM) = -5473.480903

O	-1.55971900	-2.43567400	-0.81142000
O	-2.96078800	-0.41147400	0.02689700
P	-1.42968500	-0.99015700	-0.02809700
O	-0.58086600	-0.02685800	-0.80188200
C	-2.96720000	-2.42467100	-4.75945000
C	-3.84944800	-2.37703300	-3.68477900
C	-3.37242200	-2.46508900	-2.36898800
C	-1.08133800	-2.56103700	-3.19727300

C	-1. 60245200	-2. 55561100	-4. 50462900
C	-3. 95048700	-1. 13918700	0. 69672300
C	-4. 54934800	-2. 22589800	0. 05465500
C	-5. 41076400	-3. 06545800	0. 77927200
C	-5. 75738100	-2. 76846700	2. 09160300
C	-5. 25705500	-1. 60368900	2. 66918300
C	-4. 34929600	-0. 76745200	1. 99763900
H	-0. 90732000	-2. 63905800	-5. 33477400
H	-5. 55816500	-1. 32590900	3. 67499600
C	-4. 53935600	-2. 65632600	-1. 40996000
C	-5. 67733200	-1. 94351100	-2. 21598800
H	-5. 60814900	-0. 86413200	-2. 03686500
H	-6. 67565500	-2. 27075500	-1. 90955400
H	-6. 89197000	-4. 13897500	-0. 38546900
H	-5. 78235000	-5. 19425600	0. 48303100
C	-1. 99939900	-2. 47449300	-2. 12925100
H	-3. 33016300	-2. 38121100	-5. 78339600
H	-6. 42239300	-3. 41865300	2. 65446800
C	-5. 35756300	-2. 24867800	-3. 69605100
H	-5. 70768900	-1. 46369700	-4. 37653700
H	-5. 83356000	-3. 18306100	-4. 02498600
C	-5. 84695400	-4. 24504300	-0. 06120700
C	-4. 87675100	-4. 17819600	-1. 25783700
H	-3. 95388200	-4. 71780900	-1. 01606400
H	-5. 28520100	-4. 61004000	-2. 17692500
C	-3. 95505800	0. 50668500	2. 68245600
C	-3. 12709100	0. 47909100	3. 82967500
C	-4. 56781000	1. 71873500	2. 27594300
C	-2. 50557600	-0. 71954400	4. 30440900
C	-2. 88971500	1. 69887700	4. 57021400
C	-4. 31968900	2. 93099000	3. 02431300
C	-1. 71483700	-0. 71584100	5. 42245900
H	-2. 63753100	-1. 63385800	3. 74122300
C	-2. 05919300	1. 65783300	5. 73416800
C	-3. 48593300	2. 88861500	4. 14522700
C	-1. 48995700	0. 48562100	6. 15224100
H	-1. 23074100	-1. 63501600	5. 73785400
H	-1. 89333600	2. 58364200	6. 28064700
H	-3. 30969700	3. 80220400	4. 71015200
H	-0. 85681500	0. 46756400	7. 03535500
C	0. 39667100	-2. 69769100	-3. 01471100
C	1. 26825000	-1. 73375000	-3. 58528800
C	0. 93378700	-3. 83882600	-2. 36588900
C	0. 79983800	-0. 55359100	-4. 24995600

C	2.69910800	-1.92746200	-3.51355300
C	2.36748400	-3.99881300	-2.26776600
C	1.66519900	0.33634000	-4.83508600
H	-0.26678800	-0.37169700	-4.29277100
C	3.56920000	-0.97240800	-4.12864600
C	3.20974200	-3.04778700	-2.85207700
C	3.07281900	0.12418200	-4.78163700
H	1.27201400	1.20755800	-5.35386700
H	4.64131300	-1.14633800	-4.07354000
H	4.28707700	-3.18352400	-2.78828700
H	3.74597600	0.82871000	-5.26379300
C	-6.08889200	2.97792100	0.83225300
H	-6.78887500	3.00201100	0.00080700
C	-5.47955600	1.79850600	1.17444100
H	-5.69826700	0.89843400	0.61131700
C	-5.82172200	4.17342900	1.55814200
H	-6.31228700	5.10031400	1.27213700
C	-4.95909300	4.14521000	2.62085300
H	-4.75441200	5.04733200	3.19326700
C	0.66942300	-5.96520900	-1.19164400
H	0.02286500	-6.73612900	-0.78167700
C	2.08085900	-6.09457300	-1.06278600
H	2.49824100	-6.95504900	-0.54726000
C	2.90471100	-5.13953600	-1.59204700
H	3.98407000	-5.22227400	-1.50130900
C	0.11777400	-4.88064600	-1.82075900
H	-0.95888400	-4.80678300	-1.91141300
C	-0.06199200	4.06033000	-1.73481100
C	0.05297200	4.62555900	-0.27690900
H	0.87323800	5.34290900	-0.30767600
H	-0.84797200	5.22487800	-0.09228800
C	0.22475600	3.68542500	0.90817500
C	1.17516500	3.19222600	-2.07021200
H	2.04340000	3.80708000	-1.83822600
H	1.19759100	2.96868700	-3.14345200
N	1.32782900	1.92935000	-1.33086600
C	2.47683500	1.42437600	-0.91670300
N	2.52728300	0.31944900	-0.16622000
C	3.70831900	-0.14774400	0.49124100
C	4.33148600	0.65880900	1.44532800
C	4.19562500	-1.42487500	0.21759200
C	5.47688000	0.19984500	2.09479300
C	5.33684900	-1.87547200	0.88156300
H	3.67666400	-2.05497500	-0.49407200

C	5.98631000	-1.06807800	1.81559300
H	6.86841900	-1.42862800	2.33036200
C	5.84579600	-3.26231800	0.57828400
C	6.18490200	1.09945400	3.07450100
F	6.02016200	-3.43875200	-0.75810800
F	4.98060100	-4.21259400	0.98206800
F	7.03175900	-3.51001400	1.17023100
F	6.81180800	0.39539500	4.03833200
F	5.32984400	1.95485100	3.67590900
F	7.12613400	1.85237000	2.45777600
S	4.05792000	2.15667000	-1.32281900
H	3.90641000	1.62207200	1.70220000
H	1.67960700	-0.24925800	-0.01493500
H	0.48849400	1.35287900	-1.12757700
C	1.29887000	3.71879700	1.73042300
H	3.64512600	2.68951400	-2.48775200
N	-1.07108400	-1.36388100	1.49816900
S	0.36366800	-1.84721000	1.95997900
O	0.83545800	-1.16064700	3.16766600
O	1.33479400	-1.98408600	0.83952600
C	0.05048700	-3.60410500	2.50928400
F	-0.81577400	-3.62002800	3.53463700
F	1.19840500	-4.16035500	2.91252700
F	-0.45652000	-4.33017500	1.50887100
C	-1.40215100	3.38027300	-2.07040700
C	-2.61437600	3.97130400	-1.67406600
C	-1.47923300	2.24888900	-2.89433800
C	-3.84255300	3.45159900	-2.07461200
H	-2.61136600	4.85165600	-1.03914300
C	-2.70820300	1.71945700	-3.29447300
H	-0.57984300	1.74363100	-3.22672200
C	-3.89680000	2.32038200	-2.89001600
H	-4.75776100	3.92820900	-1.73702400
H	-2.72935700	0.82822100	-3.91610500
H	-4.85477300	1.91149900	-3.20030800
C	-0.00365400	5.30207600	-2.73463000
H	-0.18107900	4.89944000	-3.74031600
H	-0.88576700	5.90299900	-2.50407100
C	1.23939200	6.17955200	-2.77933700
C	1.34999100	7.35507900	-2.12036600
C	-0.97656800	2.81424000	1.19746800
H	-1.86228500	3.44159100	1.36485900
H	-1.22826800	2.15621500	0.36072700
H	-0.85211800	2.18845000	2.08111500

C	2.35332400	5.70760000	-3.71107200
H	2.66071700	6.49414800	-4.40906700
H	3.26022800	5.39419000	-3.17478100
H	2.02513700	4.85953900	-4.31955700
C	1.39960900	2.84252700	2.97333900
H	2.42575500	2.83276500	3.35938500
H	0.76356500	3.22073900	3.78541800
H	1.10676200	1.80170800	2.80485300
C	2.58464300	8.22666900	-2.20962600
H	2.90294100	8.54173800	-1.20693900
H	3.43597200	7.73943700	-2.68807800
H	2.36849800	9.14993200	-2.76684300
C	2.48699100	4.64804700	1.58688000
H	3.42678400	4.08054700	1.53069800
H	2.45438900	5.30766000	0.71766900
H	2.57591700	5.28318600	2.48032300
C	0.28110500	7.97071800	-1.24606000
H	0.11356200	9.01596500	-1.54010200
H	-0.67948800	7.45549100	-1.28421700
H	0.60050800	7.99360500	-0.19494300

INT-16' -11

0 imaginary frequency

H = -5472.497161

G = -5472.714391

E(M06-2X-DCM) = -5473.478485

O	0.98994600	-2.97214300	-0.23450000
O	2.95850500	-1.30549000	0.01269500
P	1.32444100	-1.37108900	-0.04774100
O	0.78740600	-0.79564900	1.21128500
C	2.16248600	-5.38041500	2.97850300
C	3.03970200	-5.10724500	1.93367600
C	2.61891800	-4.35461300	0.82798600
C	0.41673800	-4.09080500	1.84701400
C	0.85638300	-4.89227800	2.91359600
C	3.73600400	-1.77695100	-1.04041800
C	3.93731100	-3.14847400	-1.19605700
C	4.55767000	-3.61566000	-2.36536100
C	5.08308700	-2.72459000	-3.29574500
C	5.00861500	-1.35446600	-3.03970400
C	4.33429800	-0.84894100	-1.91649000
H	0.15587000	-5.11642600	3.71318400
H	5.46942300	-0.64964200	-3.72582500
C	3.70757500	-4.31760000	-0.23800500

C	4. 97341100	-4. 54965700	0. 65923300
H	5. 27827200	-3. 58875800	1. 08962200
H	5. 82144100	-4. 94478300	0. 09131800
H	5. 54579900	-5. 54258200	-2. 22133000
H	4. 21824000	-5. 51911600	-3. 37653800
C	1. 33712100	-3. 81130300	0. 81810000
H	2. 48396600	-5. 96478200	3. 83703500
H	5. 56795500	-3. 08536400	-4. 19949100
C	4. 49571300	-5. 49114400	1. 78642000
H	5. 06308200	-5. 36116000	2. 71506000
H	4. 60098900	-6. 54658100	1. 49736300
C	4. 54396100	-5. 12950000	-2. 40509900
C	3. 56706500	-5. 49052000	-1. 26316700
H	2. 53938900	-5. 50270900	-1. 64380600
H	3. 76904300	-6. 46704900	-0. 81119300
C	4. 35201500	0. 62247100	-1. 63569300
C	3. 70267600	1. 53542700	-2. 50183400
C	5. 10559900	1. 10452900	-0. 53371700
C	2. 91040600	1. 11536600	-3. 61771300
C	3. 81493400	2. 95684800	-2. 25934900
C	5. 19828100	2. 52755200	-0. 29833300
C	2. 29832300	2. 02487900	-4. 44034700
H	2. 77352300	0. 05541800	-3. 78905500
C	3. 15634700	3. 87280400	-3. 13871900
C	4. 55677600	3. 41343200	-1. 16768200
C	2. 42495300	3. 42352000	-4. 20473000
H	1. 69155600	1. 67553600	-5. 27035700
H	3. 24854400	4. 93661600	-2. 93294300
H	4. 63569300	4. 48292100	-0. 98947700
H	1. 93085900	4. 12834900	-4. 86852800
C	-1. 00207700	-3. 60998500	1. 82434600
C	-1. 44472500	-2. 63893000	2. 75365600
C	-1. 92121400	-4. 19692900	0. 92019500
C	-0. 55941400	-1. 98814000	3. 67376500
C	-2. 83986900	-2. 26128800	2. 78450400
C	-3. 30967200	-3. 79899600	0. 95085400
C	-1. 01604600	-1. 06677400	4. 57967200
H	0. 49771700	-2. 21624300	3. 62477300
C	-3. 28128600	-1. 30048300	3. 75135800
C	-3. 73276600	-2. 84748000	1. 88379300
C	-2. 39974900	-0. 72662900	4. 63217300
H	-0. 31598000	-0. 57994400	5. 25260600
H	-4. 34219400	-1. 05996400	3. 78785200
H	-4. 78434700	-2. 56765800	1. 91693700

H	-2.75254400	-0.02129300	5.38166900
C	6.52816400	0.74147600	1.42366400
H	7.05156800	0.06032200	2.08921700
C	5.81557200	0.24362300	0.36442500
H	5.78898600	-0.82638900	0.19559600
C	6.59388400	2.14291300	1.66341400
H	7.16174900	2.51920300	2.51020700
C	5.95095500	3.00779900	0.81970000
H	5.99553100	4.08179900	0.98234500
C	-2.45491100	-5.76398800	-0.87757100
H	-2.13754800	-6.52676200	-1.58353300
C	-3.81910000	-5.35776400	-0.85190100
H	-4.52989600	-5.81235700	-1.53691400
C	-4.23074800	-4.40414000	0.03995200
H	-5.27105200	-4.08911800	0.07436500
C	-1.54187000	-5.20523000	-0.02229000
H	-0.50847200	-5.53060100	-0.05168200
N	0.91450900	-0.72952900	-1.49261500
S	-0.58539700	-0.56759600	-1.91574800
O	-1.00304900	0.87711100	-2.01285900
O	-1.57479300	-1.43554000	-1.25200500
C	-0.59197700	-1.11115100	-3.70015300
F	-1.82475400	-0.93514800	-4.19528000
F	-0.27247400	-2.40387500	-3.77893600
F	0.26972600	-0.40405200	-4.43906200
C	-5.28104700	1.65651700	-0.59798300
C	-5.04758700	3.07881500	-1.23793100
H	-5.14161400	3.79829800	-0.42096600
H	-5.91445500	3.26473100	-1.88724400
C	-3.79614900	3.38140400	-2.05166600
C	-4.24867800	1.36463300	0.52291000
H	-4.42643500	2.08118400	1.32544900
H	-4.42410300	0.36629300	0.93577600
N	-2.82738700	1.48715100	0.16110100
C	-1.87515400	2.02044200	0.91159900
N	-0.67029700	2.27248500	0.39188400
C	0.47828200	2.76888600	1.09847700
C	1.08122600	2.01672800	2.10783300
C	1.00175000	4.00318300	0.71634500
C	2.19759300	2.53621000	2.76178400
C	2.13177800	4.49982200	1.36885300
H	0.54162100	4.56284000	-0.09050500
C	2.72571500	3.77610900	2.40199700
H	3.60181200	4.16216600	2.90793100

C	2. 66920800	5. 85345300	0. 98915900
C	2. 87552900	1. 70333400	3. 82183100
F	2. 48269600	6. 11635700	-0. 32504600
F	2. 06140200	6. 84675800	1. 67663600
F	3. 99514800	5. 95906200	1. 23785900
F	3. 69978000	0. 78419000	3. 28840500
F	3. 61381300	2. 47041900	4. 65754200
F	1. 97096800	1. 03964300	4. 57906700
S	-2. 17651900	2. 50296100	2. 60252600
H	0. 71296800	1. 02362400	2. 33280700
H	-0. 53990200	1. 96134900	-0. 58534700
H	-2. 51715100	1. 15599200	-0. 76073000
C	-2. 88943200	4. 31903200	-1. 69301200
H	-2. 74406400	1. 32428200	2. 95782000
C	-6. 66960700	1. 78319900	0. 15924000
H	-7. 43545300	1. 92177600	-0. 61295000
H	-6. 63755300	2. 72327600	0. 71532900
C	-5. 37345900	0. 55032500	-1. 66240700
C	-4. 57058300	-0. 59594300	-1. 64188000
C	-6. 32221400	0. 65795000	-2. 69677500
C	-4. 69240900	-1. 58841100	-2. 62082200
H	-3. 81896100	-0. 75125800	-0. 87781200
C	-6. 45666200	-0. 33225800	-3. 66640300
H	-6. 97015100	1. 52854700	-2. 75338800
C	-5. 63790300	-1. 46418900	-3. 63461300
H	-4. 03421000	-2. 44988400	-2. 57313000
H	-7. 20070700	-0. 21704000	-4. 45060100
H	-5. 73609500	-2. 23420900	-4. 39505900
C	-7. 11736900	0. 64891000	1. 07216200
C	-7. 10977000	0. 74537100	2. 42230600
C	-7. 64800900	-0. 57510900	0. 34594200
H	-6. 84079200	-1. 22399600	-0. 01497800
H	-8. 31543800	-1. 17977000	0. 96262300
H	-8. 21027400	-0. 27336200	-0. 54462500
C	-7. 57564900	-0. 36088400	3. 34796600
H	-8. 50680000	-0. 07420300	3. 85813400
H	-7. 74490300	-1. 31826800	2. 85439800
H	-6. 83515800	-0. 52904600	4. 14217900
C	-3. 67024500	2. 65942900	-3. 38135400
H	-3. 20255700	1. 67257800	-3. 28344000
H	-4. 65533500	2. 49748000	-3. 82984200
H	-3. 07060900	3. 22752400	-4. 09666100
C	-1. 68773600	4. 63525000	-2. 57331300
H	-1. 14171200	3. 73557000	-2. 87610600

H	-1.98197200	5.16087200	-3.49243600
H	-0.98253700	5.29146000	-2.05109000
C	-2.94638000	5.17611900	-0.44793200
H	-3.81164700	4.99965100	0.19330600
H	-2.04675200	5.03344300	0.16758700
H	-2.95388200	6.24014300	-0.72420400
C	-6.65994700	1.95695300	3.21284700
H	-7.42940400	2.23237900	3.94722700
H	-5.75554900	1.72879300	3.79573300
H	-6.44967700	2.84406200	2.61332600

INT-16' -12

0 imaginary frequency

H = -5472.497162

G = -5472.714401

E(M06-2X-DCM) = -5473.478485

O	0.98900900	-2.97175600	-0.23452700
O	2.95869400	-1.30651900	0.01317900
P	1.32459900	-1.37097800	-0.04709800
O	0.78808000	-0.79574200	1.21223100
C	2.16004200	-5.38195200	2.97760600
C	3.03745000	-5.10890000	1.93291000
C	2.61714700	-4.35563300	0.82746900
C	0.41509900	-4.09090000	1.84653300
C	0.85422500	-4.89303000	2.91283200
C	3.73577700	-1.77810000	-1.04018700
C	3.93631600	-3.14969400	-1.19620000
C	4.55638500	-3.61692600	-2.36563600
C	5.08226400	-2.72589500	-3.29580100
C	5.00846000	-1.35579900	-3.03945000
C	4.33441100	-0.85018100	-1.91610100
H	0.15354500	-5.11706300	3.71230800
H	5.46956900	-0.65105100	-3.72544600
C	3.70587800	-4.31893700	-0.23847000
C	4.97154100	-4.55201200	0.65873300
H	5.27695000	-3.59142700	1.08943400
H	5.81936100	-4.94744900	0.09072000
H	5.54342000	-5.54444500	-2.22206000
H	4.21592400	-5.51993200	-3.37731900
C	1.33567500	-3.81155000	0.81774200
H	2.48116100	-5.96681700	3.83593300
H	5.56695000	-3.08669000	-4.19963800
C	4.49325300	-5.49358100	1.78560300
H	5.06064100	-5.36419700	2.71431500

H	4. 59795600	-6. 54898800	1. 49623300
C	4. 54182300	-5. 13074700	-2. 40576600
C	3. 56468500	-5. 49149600	-1. 26395900
H	2. 53701000	-5. 50296600	-1. 64462200
H	3. 76606700	-6. 46827000	-0. 81224600
C	4. 35261800	0. 62119800	-1. 63520900
C	3. 70394300	1. 53439100	-2. 50161900
C	5. 10590900	1. 10298700	-0. 53291800
C	2. 91178700	1. 11463000	-3. 61768900
C	3. 81673600	2. 95577400	-2. 25917600
C	5. 19907900	2. 52598300	-0. 29755800
C	2. 30034500	2. 02437100	-4. 44055000
H	2. 77444700	0. 05473900	-3. 78901100
C	3. 15885400	3. 87198200	-3. 13881300
C	4. 55835700	3. 41209400	-1. 16724500
C	2. 42756800	3. 42296700	-4. 20501300
H	1. 69362600	1. 67524700	-5. 27069200
H	3. 25145900	4. 93576000	-2. 93306400
H	4. 63770500	4. 48155700	-0. 98909000
H	1. 93397600	4. 12797900	-4. 86899100
C	-1. 00340900	-3. 60916700	1. 82405100
C	-1. 44539900	-2. 63815400	2. 75371700
C	-1. 92295900	-4. 19521400	0. 91974000
C	-0. 55962600	-1. 98824400	3. 67400600
C	-2. 84029900	-2. 25963400	2. 78475600
C	-3. 31116300	-3. 79640700	0. 95059000
C	-1. 01561200	-1. 06687000	4. 58022900
H	0. 49735300	-2. 21701400	3. 62487800
C	-3. 28105100	-1. 29888400	3. 75197100
C	-3. 73361200	-2. 84494600	1. 88388100
C	-2. 39909700	-0. 72586600	4. 63292000
H	-0. 31519200	-0. 58068000	5. 25325800
H	-4. 34180900	-1. 05772900	3. 78863500
H	-4. 78501300	-2. 56446100	1. 91717600
H	-2. 75140000	-0. 02055200	5. 38266700
C	6. 52733200	0. 73944000	1. 42520200
H	7. 05008000	0. 05809700	2. 09107600
C	5. 81508900	0. 24183400	0. 36561500
H	5. 78814300	-0. 82817600	0. 19683700
C	6. 59352900	2. 14086500	1. 66491400
H	7. 16113600	2. 51695700	2. 51196900
C	5. 95140900	3. 00597700	0. 82081800
H	5. 99636700	4. 07996900	0. 98341200
C	-2. 45770900	-5. 76131100	-0. 87855100

H	-2.14085700	-6.52404500	-1.58478600
C	-3.82164400	-5.35424100	-0.85267600
H	-4.53275900	-5.80815300	-1.53781100
C	-4.23265500	-4.40066100	0.03951800
H	-5.27276500	-4.08501200	0.07409100
C	-1.54428200	-5.20342200	-0.02311400
H	-0.51108700	-5.52942300	-0.05265700
N	0.91503700	-0.72838500	-1.49162900
S	-0.58463100	-0.56636800	-1.91550800
O	-1.00182300	0.87839000	-2.01371400
O	-1.57460200	-1.43342100	-1.25141400
C	-0.59083800	-1.11131700	-3.69950100
F	0.27102600	-0.40479300	-4.43876700
F	-1.82348900	-0.93573400	-4.19507000
F	-0.27126800	-2.40409700	-3.77713800
C	-5.28046500	1.65706300	-0.59780500
C	-5.04665100	3.07995600	-1.23628200
H	-5.14072700	3.79864000	-0.41862000
H	-5.91337500	3.26668200	-1.88556400
C	-3.79507100	3.38326500	-2.04953500
C	-4.24816100	1.36378600	0.52280600
H	-4.42585200	2.07943500	1.32614400
H	-4.42364100	0.36499400	0.93454000
N	-2.82685600	1.48657900	0.16119300
C	-1.87479200	2.02023900	0.91165900
N	-0.66994900	2.27233300	0.39200300
C	0.47869100	2.76870900	1.09845800
C	1.08131900	2.01683800	2.10821800
C	1.00259500	4.00265100	0.71578800
C	2.19788600	2.53621500	2.76192700
C	2.13275400	4.49921700	1.36813300
H	0.54271100	4.56210100	-0.09134500
C	2.72644300	3.77576600	2.40159700
H	3.60267500	4.16171400	2.90737200
C	2.67053500	5.85255100	0.98789100
C	2.87537400	1.70345300	3.82234900
F	3.99643600	5.95803800	1.23682700
F	2.48434600	6.11485800	-0.32648700
F	2.06274400	6.84630900	1.67474200
F	3.61546200	2.47024900	4.65671700
F	1.97031300	1.04197500	4.58095600
F	3.69775700	0.78243700	3.28928400
S	-2.17640200	2.50306900	2.60249500
H	0.71268300	1.02400300	2.33375500

H	-0.53965100	1.96163500	-0.58540700
H	-2.51637300	1.15459100	-0.76024400
C	-2.88872800	4.32098300	-1.69019400
H	-2.74290900	1.32400700	2.95827000
C	-6.66900500	1.78332800	0.15950900
H	-7.43475200	1.92318800	-0.61254900
H	-6.63660700	2.72268500	0.71679600
C	-5.37318800	0.55195900	-1.66334100
C	-4.57080900	-0.59467900	-1.64385100
C	-6.32183600	0.66094800	-2.69767500
C	-4.69297800	-1.58614600	-2.62376400
H	-3.81932000	-0.75107200	-0.87987100
C	-6.45662000	-0.32826300	-3.66827100
H	-6.96942600	1.53185600	-2.75348500
C	-5.63832600	-1.46056000	-3.63751900
H	-4.03517800	-2.44797000	-2.57685300
H	-7.20056200	-0.21197900	-4.45241000
H	-5.73677800	-2.22981100	-4.39871000
C	-7.11726600	0.64807300	1.07096800
C	-7.10965600	0.74282900	2.42123000
C	-7.64844000	-0.57487400	0.34328000
H	-8.31747500	-1.17900900	0.95875000
H	-8.20911400	-0.27195200	-0.54787300
H	-6.84156500	-1.22461700	-0.01688900
C	-7.57606700	-0.36443100	3.34542900
H	-6.83572100	-0.53393700	4.13948900
H	-8.50714600	-0.07802900	3.85589000
H	-7.74565900	-1.32109900	2.85059100
C	-3.66876700	2.66214400	-3.37964500
H	-3.20094200	1.67530900	-3.28217600
H	-4.65371000	2.50031700	-3.82848600
H	-3.06903200	3.23073500	-4.09447300
C	-1.68708900	4.63825000	-2.57021400
H	-1.98150300	5.16459900	-3.48887600
H	-0.98207400	5.29422000	-2.04744300
H	-1.14083700	3.73898800	-2.87382700
C	-2.94606500	5.17730500	-0.44461000
H	-2.04638700	5.03455700	0.17083300
H	-2.95392500	6.24150700	-0.72018100
H	-3.81128200	5.00011600	0.19649500
C	-6.65938400	1.95322900	3.21331900
H	-7.42882800	2.22813000	3.94791200
H	-5.75518500	1.72392300	3.79606300
H	-6.44859500	2.84096200	2.61490200

INT-16' -13

0 imaginary frequency

H = -5472.494358

G = -5472.713090

E(M06-2X-DCM) = -5473.482807

O	-1.26875100	-1.98263500	-1.61746700
O	-2.87123000	-0.65476500	-0.05955000
P	-1.28685300	-0.99329300	-0.29771800
O	-0.55985500	0.28943300	-0.56999000
C	-2.73643100	-0.47811800	-5.24399900
C	-3.60009200	-0.97975100	-4.27543000
C	-3.09412200	-1.55565700	-3.10093700
C	-0.82096400	-1.04619000	-3.82156000
C	-1.36158300	-0.55299100	-5.02374300
C	-3.76414700	-1.69571400	0.21765800
C	-4.25092800	-2.47402800	-0.83508500
C	-5.00291000	-3.62527100	-0.55051600
C	-5.35890500	-3.93815800	0.75563900
C	-4.97841000	-3.07328100	1.77940600
C	-4.17712600	-1.94345100	1.54320000
H	-0.67576400	-0.20576300	-5.79079100
H	-5.29037800	-3.27296700	2.80031000
C	-4.21657100	-2.25409000	-2.34521100
C	-5.44078100	-1.39981100	-2.81899900
H	-5.49178200	-0.49254500	-2.20561900
H	-6.39048300	-1.93218300	-2.70851000
H	-6.37327500	-4.27167600	-2.10248100
H	-5.14007200	-5.46590300	-1.71271100
C	-1.72451200	-1.51445800	-2.84396600
H	-3.11943300	-0.05134400	-6.16770200
H	-5.93987600	-4.82973800	0.97780600
C	-5.11299500	-1.02445000	-4.28090900
H	-5.56091500	-0.07126000	-4.58523500
H	-5.48537100	-1.78343600	-4.98308700
C	-5.31817100	-4.38948500	-1.81734100
C	-4.37952600	-3.72871700	-2.84717900
H	-3.39864400	-4.21701500	-2.82011000
H	-4.75124300	-3.78230500	-3.87530700
C	-3.90285700	-1.03886700	2.70652400
C	-3.06636000	-1.46651700	3.76494800
C	-4.62979000	0.17301500	2.81879600
C	-2.32612400	-2.69063100	3.71799600
C	-2.94207700	-0.65062700	4.95297700

C	-4.49344700	0.97995300	4.01094500
C	-1.53090400	-3.08145700	4.76211000
H	-2.37111300	-3.29347500	2.82067400
C	-2.10308200	-1.09780200	6.02186400
C	-3.65291500	0.54886600	5.04090100
C	-1.41942200	-2.27997500	5.93334700
H	-0.95634400	-3.99922400	4.68225000
H	-2.02405400	-0.47373800	6.90931600
H	-3.56152500	1.15557600	5.94000900
H	-0.78111200	-2.60707900	6.74982400
C	0.66597500	-1.08310900	-3.66576600
C	1.41323000	0.12010000	-3.75802000
C	1.33960500	-2.32415900	-3.53225000
C	0.80395800	1.41095700	-3.88754800
C	2.85794300	0.07215900	-3.72794000
C	2.78363700	-2.35200600	-3.46321200
C	1.55314400	2.55268200	-4.02364200
H	-0.27695900	1.47715300	-3.88609400
C	3.60431900	1.28512800	-3.86616200
C	3.50302900	-1.15805800	-3.57336500
C	2.97640200	2.49235100	-4.02073800
H	1.05567000	3.51234600	-4.14188000
H	4.68999300	1.22213300	-3.85615800
H	4.58977500	-1.18893600	-3.53709600
H	3.55770300	3.40238600	-4.14775900
C	-6.26726100	1.78196300	1.97445100
H	-6.96826900	2.09012400	1.20285300
C	-5.54955000	0.62459200	1.81828800
H	-5.68554700	0.02554400	0.92513700
C	-6.11135000	2.58412900	3.14042800
H	-6.68780200	3.49944500	3.24774300
C	-5.24651100	2.19051600	4.12599300
H	-5.12553700	2.78598400	5.02828500
C	1.33737500	-4.76132000	-3.35663600
H	0.78916100	-5.69881300	-3.32535000
C	2.75623800	-4.77668600	-3.24715500
H	3.27686600	-5.72205100	-3.12226800
C	3.45770800	-3.60386100	-3.30487600
H	4.54084000	-3.59783400	-3.22207600
C	0.65610600	-3.58112300	-3.49588000
H	-0.42328900	-3.59517000	-3.58264600
C	-0.45587800	4.46117300	0.23935500
C	-0.36772500	4.38796100	1.80997400
H	0.41526400	5.09354500	2.09639800

H	-1.29818300	4.82102600	2.20068700
C	-0.14599100	3.05772300	2.51482800
C	0.83866400	3.90188400	-0.39990500
H	1.65680300	4.45906400	0.05595200
H	0.84348600	4.12079600	-1.47286400
N	1.13263800	2.47323600	-0.20609800
C	2.33307400	1.96350200	0.00626900
N	2.50704900	0.66035300	0.25036600
C	3.73878200	0.08638200	0.69598500
C	4.28310300	0.48408100	1.91846700
C	4.35760600	-0.90413100	-0.06500700
C	5.47931000	-0.08186400	2.35786300
C	5.54955400	-1.46829700	0.39025300
H	3.90064900	-1.23240100	-0.99034900
C	6.11953500	-1.05904400	1.59588200
H	7.04218300	-1.50695100	1.94417000
C	6.20171200	-2.54226000	-0.44366700
C	6.09909300	0.39711500	3.64506900
F	6.37232700	-2.12910400	-1.72738900
F	5.45198800	-3.66015500	-0.49579500
F	7.41707900	-2.88582700	0.02863700
F	6.96177000	1.41702500	3.42469800
F	6.79359300	-0.58101800	4.26051400
F	5.16661600	0.85087200	4.51038700
S	3.82448500	2.95250600	-0.01558500
H	3.75996600	1.20485400	2.53607000
H	1.72665700	-0.00325800	0.12801800
H	0.36293100	1.78055500	-0.27561800
C	0.91226900	2.81487800	3.32250500
H	3.35837500	3.85072700	-0.90344300
N	-0.87027400	-1.93084900	0.94480100
S	0.61393600	-2.41304100	1.21113000
O	1.02133600	-2.25529300	2.61142200
O	1.58078500	-1.96307100	0.17203200
C	0.50028600	-4.25969300	0.95853900
F	1.70709400	-4.81146900	1.12834900
F	0.06161300	-4.54376300	-0.27118100
F	-0.34528000	-4.79717200	1.85179500
C	-1.74974000	3.87581500	-0.34805700
C	-2.99326700	4.21240600	0.21567700
C	-1.76151900	3.08571100	-1.50458800
C	-4.18952600	3.78034100	-0.35046700
H	-3.03868700	4.82492900	1.11102100
C	-2.95866900	2.64396100	-2.07438800

H	-0.83535500	2.78685600	-1.98062200
C	-4.17901700	2.99298100	-1.50333500
H	-5.13059600	4.05238000	0.11818000
H	-2.92799500	2.01600300	-2.96077600
H	-5.11181400	2.65087400	-1.94366800
C	-0.42097800	6.01756900	-0.08753000
H	-1.28828300	6.45288000	0.42285200
H	0.45817200	6.42892900	0.41812400
C	-0.44610000	6.46181400	-1.54291700
C	0.66173300	6.83954400	-2.22124100
C	-1.28054200	2.06852800	2.36987500
H	-1.14698600	1.17417900	2.97833000
H	-2.22690800	2.53362100	2.67522000
H	-1.42521500	1.74325600	1.33528800
C	-1.82286100	6.53049800	-2.19076500
H	-2.02134800	5.67302700	-2.84493200
H	-2.60980400	6.52537500	-1.43285500
H	-1.94723100	7.43969200	-2.78759700
C	1.06276900	1.50727600	4.09127700
H	0.37060800	1.45674700	4.94275300
H	0.87883000	0.61576900	3.48380300
H	2.07414700	1.41485200	4.50394500
C	0.62211800	7.28543200	-3.66843600
H	-0.31845800	7.05646300	-4.17147700
H	0.79466200	8.36878900	-3.75054300
H	1.42796400	6.80407900	-4.23927800
C	2.02903800	3.79107000	3.63072100
H	1.95577500	4.75414300	3.12196300
H	2.06061300	3.99253900	4.71122400
H	3.00987000	3.36323300	3.37923000
C	2.06384400	6.89584900	-1.65411500
H	2.70613100	6.12830600	-2.11351600
H	2.53008000	7.86019100	-1.89776300
H	2.11802400	6.77280300	-0.57056700

INT-16⁷-14

0 imaginary frequency

H = -5472.493182

G = -5472.711636

E(M06-2X-DCM) = -5473.480923

O	-1.55976800	-2.43499700	-0.81248700
O	-2.96041700	-0.41104200	0.02716100
P	-1.42943200	-0.98999400	-0.02822800
O	-0.58055600	-0.02628300	-0.80149500

C	-2.96745700	-2.42137200	-4.76043500
C	-3.84963800	-2.37401900	-3.68570000
C	-3.37258700	-2.46297900	-2.36997400
C	-1.08157800	-2.55922800	-3.19842100
C	-1.60273800	-2.55292400	-4.50574100
C	-3.95019800	-1.13898300	0.69665800
C	-4.54941300	-2.22506000	0.05386500
C	-5.41099400	-3.06489500	0.77796200
C	-5.75735200	-2.76876200	2.09055800
C	-5.25658800	-1.60457800	2.66894600
C	-4.34866800	-0.76809700	1.99791400
H	-0.90767500	-2.63618100	-5.33596300
H	-5.55746000	-1.32748000	3.67501900
C	-4.53957900	-2.65447700	-1.41104000
C	-5.67734900	-1.94081500	-2.21658700
H	-5.60784500	-0.86157000	-2.03678700
H	-6.67576300	-2.26795700	-1.91034300
H	-6.89258000	-4.13704700	-0.38752400
H	-5.78335300	-5.19336500	0.48022200
C	-1.99955600	-2.47294500	-2.13029000
H	-3.33044500	-2.37723500	-5.78434400
H	-6.42248600	-3.41916600	2.65302600
C	-5.35771000	-2.24515200	-3.69684900
H	-5.70757400	-1.45960300	-4.37681800
H	-5.83403800	-3.17915000	-4.02639100
C	-5.84760300	-4.24374100	-0.06333400
C	-4.87740000	-4.17636900	-1.25993300
H	-3.95467200	-4.71638500	-1.01852200
H	-5.28597900	-4.60748400	-2.17930400
C	-3.95382300	0.50533700	2.68364900
C	-3.12594200	0.47644400	3.83091000
C	-4.56582200	1.71804300	2.27796500
C	-2.50502600	-0.72286100	4.30473000
C	-2.88797100	1.69553200	4.57239400
C	-4.31708100	2.92959800	3.02725700
C	-1.71432900	-0.72042400	5.42281200
H	-2.63738500	-1.63666200	3.74081100
C	-2.05755900	1.65316200	5.73638200
C	-3.48349300	2.88592000	4.14824000
C	-1.48892000	0.48034800	6.15356800
H	-1.23067000	-1.64007800	5.73748300
H	-1.89128200	2.57846400	6.28359200
H	-3.30680000	3.79899300	4.71385700
H	-0.85585100	0.46128400	7.03671300

C	0.39638800	-2.69649600	-3.01594100
C	1.26831600	-1.73253500	-3.58593900
C	0.93309100	-3.83818800	-2.36774500
C	0.80033600	-0.55189800	-4.25006600
C	2.69911100	-1.92672900	-3.51417300
C	2.36672300	-3.99867500	-2.26958400
C	1.66603100	0.33806900	-4.83464400
H	-0.26623000	-0.36967400	-4.29293600
C	3.56956000	-0.97159900	-4.12864400
C	3.20933300	-3.04757600	-2.85326900
C	3.07358300	0.12548000	-4.78111700
H	1.27316700	1.20965000	-5.35306000
H	4.64161500	-1.14587000	-4.07349200
H	4.28662000	-3.18367200	-2.78941400
H	3.74700900	0.83008000	-5.26279000
C	-6.08586000	2.97922000	0.83491500
H	-6.78568100	3.00434300	0.00336500
C	-5.47735500	1.79917000	1.17638700
H	-5.69656900	0.89963300	0.61260600
C	-5.81805300	4.17404100	1.56169700
H	-6.30795700	5.10144800	1.27625000
C	-4.95565600	4.14450900	2.62456100
H	-4.75051300	5.04608700	3.19766600
C	0.66796500	-5.96520900	-1.19483400
H	0.02113700	-6.73620200	-0.78543000
C	2.07934600	-6.09507100	-1.06590400
H	2.49641600	-6.95597800	-0.55084600
C	2.90353900	-5.13995600	-1.59449400
H	3.98286400	-5.22305600	-1.50366600
C	0.11670500	-4.88008500	-1.82332500
H	-0.95992200	-4.80582400	-1.91402500
C	-0.06186600	4.06152600	-1.73418000
C	0.05281800	4.62642400	-0.27613700
H	0.87320700	5.34365400	-0.30653400
H	-0.84808600	5.22582800	-0.09159700
C	0.22415500	3.68594700	0.90874100
C	1.17535200	3.19349200	-2.06953600
H	2.04353100	3.80826600	-1.83713000
H	1.19804500	2.97027700	-3.14283400
N	1.32778600	1.93036500	-1.33057400
C	2.47661600	1.42507600	-0.91632100
N	2.52663700	0.31967700	-0.16648500
C	3.70737400	-0.14800600	0.49117400
C	4.33021300	0.65793200	1.44600100

C	4. 19477000	-1. 42495500	0. 21686600
C	5. 47536300	0. 19853500	2. 09557200
C	5. 33574600	-1. 87600100	0. 88096300
H	3. 67605700	-2. 05459900	-0. 49538100
C	5. 98488300	-1. 06922000	1. 81573500
H	6. 86678500	-1. 43013400	2. 33061100
C	5. 84479600	-3. 26262800	0. 57686500
C	6. 18317600	1. 09737000	3. 07614100
F	7. 03016700	-3. 51104700	1. 16970100
F	6. 02039800	-3. 43782900	-0. 75952100
F	4. 97908300	-4. 21316400	0. 97893300
F	7. 12639500	1. 84881900	2. 46065600
F	6. 80771100	0. 39258800	4. 04099400
F	5. 32847100	1. 95407000	3. 67617600
S	4. 05794500	2. 15733100	-1. 32142300
H	3. 90507800	1. 62103400	1. 70335000
H	1. 67872800	-0. 24884600	-0. 01599900
H	0. 48836900	1. 35399300	-1. 12747900
C	1. 29811200	3. 71883900	1. 73120600
H	3. 64554000	2. 69163300	-2. 48581900
N	-1. 07080400	-1. 36474200	1. 49776600
S	0. 36392800	-1. 84882100	1. 95901300
O	0. 83619300	-1. 16302500	3. 16693300
O	1. 33471000	-1. 98546300	0. 83826600
C	0. 05020200	-3. 60589000	2. 50745800
F	-0. 45726100	-4. 33122300	1. 50673400
F	-0. 81585600	-3. 62213500	3. 53298200
F	1. 19801000	-4. 16276600	2. 91016000
C	-1. 40195300	3. 38153800	-2. 07014100
C	-2. 61424400	3. 97248700	-1. 67388000
C	-1. 47890200	2. 25027700	-2. 89425700
C	-3. 84235600	3. 45281400	-2. 07467000
H	-2. 61133100	4. 85274300	-1. 03882200
C	-2. 70780900	1. 72088600	-3. 29464500
H	-0. 57946400	1. 74509200	-3. 22662600
C	-3. 89647400	2. 32172300	-2. 89025700
H	-4. 75762300	3. 92937700	-1. 73716100
H	-2. 72885300	0. 82975700	-3. 91643100
H	-4. 85439400	1. 91287500	-3. 20075200
C	-0. 00330800	5. 30349500	-2. 73374300
H	-0. 18056900	4. 90104900	-3. 73953200
H	-0. 88543900	5. 90439100	-2. 50319700
C	1. 23977700	6. 18092500	-2. 77804000
C	1. 35030700	7. 35629500	-2. 11878000

C	-0.97735100	2.81485000	1.19752000
H	-1.22827800	2.15624000	0.36099200
H	-0.85358100	2.18962500	2.08166300
H	-1.86327200	3.44220700	1.36373700
C	2.35384500	5.70914000	-3.70969300
H	2.66164400	6.49593300	-4.40722600
H	3.26052700	5.39524100	-3.17330500
H	2.02560600	4.86144600	-4.31866400
C	1.39840900	2.84203000	2.97379300
H	2.42433800	2.83237200	3.36040100
H	0.76178100	3.21964800	3.78568400
H	1.10595800	1.80120600	2.80461200
C	2.58501100	8.22785400	-2.20758400
H	2.90320200	8.54253000	-1.20473800
H	3.43637800	7.74076400	-2.68611200
H	2.36896300	9.15133600	-2.76447200
C	0.28130400	7.97177500	-1.24449600
H	0.60040600	7.99408300	-0.19327500
H	0.11409300	9.01719600	-1.53809400
H	-0.67940100	7.45679300	-1.28317700
C	2.48648000	4.64785500	1.58823700
H	2.45414500	5.30787800	0.71932700
H	2.57543400	5.28255600	2.48198500
H	3.42614000	4.08015000	1.53191900

INT-16' -15

0 imaginary frequency

H = -5472.494358

G = -5472.713090

E(M06-2X-DCM) = -5473.482797

O	-1.26889300	-1.98427600	-1.61537300
O	-2.87174900	-0.65457700	-0.05941000
P	-1.28726700	-0.99316100	-0.29697500
O	-0.56047400	0.28931200	-0.57092800
C	-2.73578800	-0.48388900	-5.24391300
C	-3.59963600	-0.98456000	-4.27501100
C	-3.09387600	-1.55913400	-3.09978600
C	-0.82058900	-1.05038200	-3.82047200
C	-1.36098600	-0.55847500	-5.02329000
C	-3.76460400	-1.69526600	0.21876700
C	-4.25100900	-2.47496600	-0.83312700
C	-5.00291100	-3.62595400	-0.54733100
C	-5.35922100	-3.93728300	0.75911200
C	-4.97917400	-3.07105000	1.78190200

C	-4.17802000	-1.94139300	1.54448500
H	-0.67502600	-0.21204200	-5.79057000
H	-5.29143700	-3.26947200	2.80296300
C	-4.21637600	-2.25683900	-2.34350800
C	-5.44060600	-1.40324400	-2.81853200
H	-5.49186700	-0.49530500	-2.20617500
H	-6.39025600	-1.93563100	-2.70766800
H	-6.37286100	-4.27452500	-2.09876900
H	-5.13945800	-5.46800300	-1.70733400
C	-1.72432900	-1.51757900	-2.84256300
H	-3.11860300	-0.05810700	-6.16815000
H	-5.94010700	-4.82868100	0.98222200
C	-5.11253200	-1.02946000	-4.28078100
H	-5.56052600	-0.07668000	-4.58627700
H	-5.48463100	-1.78928800	-4.98219400
C	-5.31778600	-4.39175200	-1.81329700
C	-4.37906400	-3.73205000	-2.84376300
H	-3.39813700	-4.22021700	-2.81599600
H	-4.75063100	-3.78687900	-3.87188100
C	-3.90441800	-1.03512900	2.70665600
C	-3.06797400	-1.46092600	3.76586500
C	-4.63193000	0.17656800	2.81708000
C	-2.32730100	-2.68484500	3.72082900
C	-2.94425300	-0.64327800	4.95273400
C	-4.49614200	0.98529200	4.00808100
C	-1.53214000	-3.07386000	4.76566400
H	-2.37194500	-3.28902100	2.82438600
C	-2.10528000	-1.08857400	6.02241900
C	-3.65558900	0.55605800	5.03879300
C	-1.42115700	-2.27061800	5.93574100
H	-0.95727000	-3.99155800	4.68727800
H	-2.02665300	-0.46319000	6.90897600
H	-3.56460100	1.16410100	5.93704100
H	-0.78287600	-2.59630000	6.75280800
C	0.66631600	-1.08726300	-3.66444800
C	1.41369900	0.11576400	-3.75800500
C	1.33981000	-2.32822700	-3.52949700
C	0.80452900	1.40654100	-3.88877800
C	2.85840200	0.06770800	-3.72798000
C	2.78384400	-2.35614800	-3.46048300
C	1.55381200	2.54805100	-4.02611800
H	-0.27638000	1.47282300	-3.88719600
C	3.60488300	1.28045700	-3.86756200
C	3.50336300	-1.16240800	-3.57208600

C	2. 97706300	2. 48757400	-4. 02333300
H	1. 05642600	3. 50765100	-4. 14524300
H	4. 69055000	1. 21736800	-3. 85757100
H	4. 59011000	-1. 19337300	-3. 53590200
H	3. 55843900	3. 39742200	-4. 15134800
C	-6. 27017500	1. 78342800	1. 97024900
H	-6. 97129000	2. 09009700	1. 19815000
C	-5. 55181600	0. 62622900	1. 81581800
H	-5. 68741400	0. 02580900	0. 92352800
C	-6. 11480200	2. 58735800	3. 13508700
H	-6. 69176500	3. 50251000	3. 24103500
C	-5. 24983500	2. 19563900	4. 12128900
H	-5. 12926600	2. 79247000	5. 02273300
C	1. 33731800	-4. 76517200	-3. 35094100
H	0. 78899200	-5. 70255900	-3. 31848900
C	2. 75618000	-4. 78056500	-3. 24149100
H	3. 27670800	-5. 72583400	-3. 11547100
C	3. 45777600	-3. 60788600	-3. 30066000
H	4. 54091200	-3. 60188900	-3. 21791300
C	0. 65617900	-3. 58506700	-3. 49159600
H	-0. 42322100	-3. 59910700	-3. 57830600
C	-0. 45488300	4. 46133800	0. 23566800
C	-0. 36690900	4. 38947800	1. 80636800
H	0. 41594500	5. 09542600	2. 09225100
H	-1. 29745800	4. 82274000	2. 19662400
C	-0. 14500500	3. 05987100	2. 51235700
C	0. 83974900	3. 90142600	-0. 40285600
H	1. 65784400	4. 45876800	0. 05290800
H	0. 84492800	4. 11962500	-1. 47595900
N	1. 13341200	2. 47285000	-0. 20797200
C	2. 33382800	1. 96312400	0. 00447900
N	2. 50775500	0. 66017700	0. 24962400
C	3. 73939700	0. 08651400	0. 69590800
C	4. 28375900	0. 48547800	1. 91796200
C	4. 35802700	-0. 90498900	-0. 06393900
C	5. 47979400	-0. 08025900	2. 35806300
C	5. 54984500	-1. 46889400	0. 39200600
H	3. 90106500	-1. 23418600	-0. 98894900
C	6. 11984300	-1. 05844000	1. 59721200
H	7. 04236800	-1. 50615700	1. 94606700
C	6. 20183000	-2. 54390100	-0. 44070400
C	6. 09955200	0. 40003900	3. 64478800
F	5. 45184400	-3. 66166100	-0. 49171900
F	7. 41706600	-2. 88724600	0. 03207700

F	6.37267700	-2.13213600	-1.72484700
F	6.79426200	-0.57737900	4.26113000
F	5.16701700	0.85442800	4.50971700
F	6.96200500	1.41991900	3.42342800
S	3.82533700	2.95195600	-0.01890800
H	3.76074800	1.20705200	2.53473000
H	1.72729100	-0.00352000	0.12823100
H	0.36353000	1.78031800	-0.27674000
C	0.91343400	2.81774700	3.32001600
H	3.35885500	3.84954800	-0.90720800
N	-0.87077800	-1.92892700	0.94693100
S	0.61332300	-2.41119700	1.21374900
O	1.02081600	-2.25178600	2.61381200
O	1.58022600	-1.96279400	0.17402900
C	0.49925700	-4.25813600	0.96347000
F	-0.34639100	-4.79431800	1.85739800
F	1.70595800	-4.80995300	1.13393900
F	0.06050300	-4.54362800	-0.26589400
C	-1.74865000	3.87548200	-0.35146000
C	-2.99224300	4.21192600	0.21225100
C	-1.76028000	3.08512300	-1.50779200
C	-4.18840500	3.77941600	-0.35372600
H	-3.03777000	4.82467500	1.10743300
C	-2.95735100	2.64292700	-2.07743100
H	-0.83405100	2.78635700	-1.98375900
C	-4.17773700	2.99175500	-1.50640100
H	-5.12952100	4.05124400	0.11493800
H	-2.92656000	2.01474400	-2.96365800
H	-5.11047200	2.64925800	-1.94655600
C	-0.41991400	6.01741500	-0.09258300
H	-1.28733800	6.45320700	0.41719800
H	0.45913100	6.42929800	0.41283300
C	-0.44477400	6.46027600	-1.54838600
C	0.66307600	6.83762600	-2.22686500
C	-1.27957300	2.07053700	2.36841000
H	-1.14620100	1.17695800	2.97803400
H	-2.22596300	2.53606000	2.67298000
H	-1.42405400	1.74398200	1.33419000
C	-1.82136500	6.52839400	-2.19677300
H	-1.94743900	7.44005800	-2.78956500
H	-2.01717200	5.67354900	-2.85516600
H	-2.60887700	6.51780100	-1.43958000
C	1.06429100	1.51081800	4.08981600
H	2.07642500	1.41789700	4.50053400

H	0.37387300	1.46196600	4.94282400
H	0.87827000	0.61881100	3.48374900
C	0.62321800	7.28268800	-3.67428000
H	0.79627200	8.36591700	-3.75699300
H	1.42860200	6.80063900	-4.24519800
H	-0.31771300	7.05399100	-4.17678100
C	2.06517500	6.89438100	-1.65978800
H	2.11932400	6.77207800	-0.57615300
H	2.70746800	6.12650600	-2.11863300
H	2.53142500	7.85854200	-1.90410100
C	2.03011700	3.79432900	3.62735000
H	1.95662900	4.75704700	3.11795600
H	2.06183600	3.99654000	4.70771000
H	3.01097800	3.36647800	3.37599500

INT-16' -2

0 imaginary frequency

H = -5472.494436

G = -5472.712517

E(M06-2X-DCM) = -5473.479237

O	-1.56180900	-2.36709800	-1.12614500
O	-3.08403600	-0.41285600	-0.34425300
P	-1.53944200	-0.94766100	-0.29411500
O	-0.67058800	0.06993300	-0.97055400
C	-2.50894400	-2.12163400	-5.19760500
C	-3.51064700	-2.16393100	-4.23278300
C	-3.18533400	-2.33264800	-2.87940800
C	-0.81181100	-2.33789100	-3.44156800
C	-1.17871600	-2.24726300	-4.79677800
C	-4.11424200	-1.20431900	0.17538500
C	-4.62106600	-2.25617600	-0.59155700
C	-5.53320800	-3.15185100	-0.01018500
C	-6.01410000	-2.94423400	1.27703100
C	-5.59634800	-1.81328100	1.97572600
C	-4.64441000	-0.92316500	1.45142000
H	-0.39089000	-2.25747100	-5.54427200
H	-6.00073000	-1.60596400	2.96216500
C	-4.44710600	-2.59800800	-2.07006300
C	-5.50364500	-1.85529000	-2.95631500
H	-5.48562100	-0.78866300	-2.70366900
H	-6.52154200	-2.22055800	-2.78822300
H	-6.86461500	-4.16881300	-1.38684100
H	-5.83292700	-5.26276200	-0.47140600
C	-1.84895600	-2.33900700	-2.48734300

H	-2.75279000	-2.00839700	-6.25103900
H	-6.71859100	-3.63856200	1.72804200
C	-5.01070400	-2.05779300	-4.40705400
H	-5.30007600	-1.23508500	-5.07120000
H	-5.42555300	-2.97575800	-4.84647100
C	-5.85746200	-4.28260300	-0.96130800
C	-4.76871000	-4.13066200	-2.04285100
H	-3.86604100	-4.67172600	-1.73668100
H	-5.07016800	-4.51172400	-3.02366000
C	-4.33661500	0.31221300	2.24312900
C	-3.60807300	0.22959400	3.45309500
C	-4.92862400	1.53879100	1.85051000
C	-3.01493800	-0.98780700	3.91602600
C	-3.44683000	1.41033300	4.27279800
C	-4.75820500	2.71145500	2.67881900
C	-2.31923800	-1.03760300	5.09460600
H	-3.09305600	-1.87302300	3.29894300
C	-2.71521100	1.31400600	5.49843100
C	-4.01887400	2.61660500	3.86102900
C	-2.16873400	0.12577900	5.90144600
H	-1.85468500	-1.96914600	5.40319100
H	-2.60689000	2.21079200	6.10455900
H	-3.90072300	3.50057600	4.48511700
H	-1.61137100	0.06575500	6.83246800
C	0.63450700	-2.46946400	-3.08440000
C	1.54827100	-1.44799200	-3.44826900
C	1.10977500	-3.65622500	-2.47017100
C	1.13937400	-0.21432100	-4.05370800
C	2.96270400	-1.63283800	-3.21010900
C	2.52145700	-3.80591400	-2.19851800
C	2.05272600	0.73395600	-4.44035600
H	0.08172600	-0.03716100	-4.20896200
C	3.88343300	-0.61927900	-3.62950700
C	3.40963300	-2.79756000	-2.58102000
C	3.44750600	0.53021100	-4.23329500
H	1.71069400	1.64839100	-4.91917700
H	4.94505800	-0.79422700	-3.46735800
H	4.47255200	-2.92120300	-2.38496700
H	4.15865700	1.28488600	-4.55854700
C	-6.34456100	2.85841100	0.35548100
H	-6.97271000	2.92151700	-0.52942300
C	-5.74827900	1.66875000	0.68319300
H	-5.90809700	0.79809500	0.05737200
C	-6.15596700	4.01479600	1.16422100

H	-6.63648800	4.95026100	0.88926400
C	-5.38126200	3.93876600	2.29004300
H	-5.23688600	4.81061800	2.92435100
C	0.74430400	-5.88031700	-1.52506700
H	0.06787200	-6.69142600	-1.26974700
C	2.13126800	-6.00759700	-1.23227000
H	2.50017300	-6.90904000	-0.75074100
C	2.99231700	-4.99875200	-1.56665500
H	4.05667300	-5.08536900	-1.36179800
C	0.25408800	-4.75036900	-2.12475600
H	-0.80375000	-4.68056300	-2.34724100
C	0.21359200	4.30380400	-1.24714000
C	0.40146400	4.74316800	0.24415600
H	1.38016700	5.22549200	0.29209900
H	-0.32190900	5.55107300	0.42160800
C	0.25497500	3.73658100	1.38261300
C	1.22848200	3.20762800	-1.66426900
H	2.21605300	3.65644700	-1.69804600
H	1.01539000	2.87941200	-2.68602300
N	1.34292000	1.98657600	-0.85137100
C	2.44786000	1.54224600	-0.27546800
N	2.53845100	0.28827500	0.17299900
C	3.71104200	-0.28888400	0.76208300
C	4.83396500	-0.50502000	-0.03383200
C	3.69134500	-0.69588100	2.09845300
C	5.96523600	-1.10868500	0.51850300
C	4.82940100	-1.29710100	2.63531100
H	2.79438000	-0.56465800	2.69486400
C	5.96966900	-1.50277900	1.85414900
H	6.84635100	-1.97299600	2.28285800
C	4.80964100	-1.78344300	4.06435500
C	7.17663400	-1.30691100	-0.35296500
F	4.32882200	-3.04026300	4.15214100
F	4.04053700	-1.00040700	4.84489400
F	6.05433800	-1.79639000	4.59600200
F	7.84621300	-0.14919200	-0.54793300
F	6.82751500	-1.76168000	-1.58481500
F	8.04474200	-2.19137400	0.17344100
S	3.90060400	2.55021500	-0.03073200
H	4.81010500	-0.22956900	-1.08227900
H	1.74409500	-0.36747000	0.08554900
H	0.55243500	1.31141200	-0.88643400
C	1.11724000	3.68513500	2.42493000
H	3.23334800	3.71724600	0.02230500

N	-1.28098400	-1.36188800	1.24438300
S	0.10201600	-1.91419000	1.76985600
O	0.51439100	-1.29612500	3.04004600
O	1.15296000	-2.02596000	0.71910100
C	-0.27843100	-3.68899300	2.21248600
F	0.83069400	-4.28359100	2.66377600
F	-0.72717900	-4.35304500	1.14480700
F	-1.21234700	-3.73663000	3.17498900
C	-1.24590500	3.95564200	-1.61060100
C	-2.27187100	4.86844800	-1.30449600
C	-1.60422500	2.81058600	-2.33411800
C	-3.58825500	4.64853800	-1.70109100
H	-2.04831900	5.77239400	-0.74525100
C	-2.92522200	2.58098100	-2.72740900
H	-0.87579600	2.04809100	-2.57868300
C	-3.92334800	3.50017100	-2.42004200
H	-4.35437300	5.37272600	-1.43843900
H	-3.16389000	1.66762900	-3.26508900
H	-4.95108000	3.32177500	-2.72292800
C	0.55231700	5.56130400	-2.17075100
H	0.27338200	5.27737600	-3.19328500
H	-0.15502700	6.34284900	-1.88660800
C	1.97036400	6.11784600	-2.20311000
C	2.38506100	7.16307400	-1.45140700
C	-1.01455700	2.91357000	1.37037100
H	-1.14012100	2.31715600	2.27347100
H	-1.88851000	3.57267500	1.29238400
H	-1.07895700	2.23376900	0.51556500
C	2.90030400	5.50452600	-3.24954900
H	2.37652100	4.76092800	-3.85674900
H	3.28361400	6.26478700	-3.94043900
H	3.77663500	5.00463300	-2.81542500
C	0.93992200	2.71520600	3.58456200
H	0.59553000	1.72370900	3.27870700
H	1.88944200	2.57945400	4.11537000
H	0.21895400	3.09341900	4.32310400
C	3.78740600	7.72603400	-1.54738200
H	4.48333000	7.08475200	-2.09138400
H	3.77781600	8.70642100	-2.04590200
H	4.20292900	7.89705200	-0.54530300
C	2.29694200	4.61136100	2.64263700
H	2.44522500	5.36372000	1.86397700
H	2.16230200	5.15673400	3.58805900
H	3.23207100	4.04532200	2.75339400

C	1.52537100	7.93508500	-0.47645500
H	1.87711500	7.79884000	0.55588600
H	1.59993000	9.01122400	-0.68546300
H	0.46955200	7.66305300	-0.50107400

INT-16' -3

0 imaginary frequency

H = -5472.494464

G = -5472.709815

E(M06-2X-DCM) = -5473.475920

O	-2.14815700	-1.71953700	-1.13139500
O	-3.08973900	0.44130900	-0.05122800
P	-1.69321600	-0.35645400	-0.35176800
O	-0.85589300	0.56963900	-1.17910700
C	-4.40805000	-1.56469900	-4.65121500
C	-5.02741000	-1.51773800	-3.40703500
C	-4.27643900	-1.61473800	-2.22469800
C	-2.22978600	-1.73761400	-3.55343100
C	-3.02114000	-1.69353500	-4.71326300
C	-4.08053600	-0.07264200	0.79423300
C	-4.88694900	-1.12835900	0.37135000
C	-5.68821500	-1.78758300	1.31743400
C	-5.81369300	-1.29482200	2.61052000
C	-5.14183800	-0.12226800	2.95383400
C	-4.25330200	0.50533400	2.06747300
H	-2.52465500	-1.74327900	-5.67801200
H	-5.27652800	0.31131700	3.94049600
C	-5.20174700	-1.68937900	-1.01557100
C	-6.46615400	-0.96339600	-1.59917800
H	-6.32205300	0.11920700	-1.50379700
H	-7.38210400	-1.22471300	-1.06160700
H	-7.39604900	-2.90830900	0.56757300
H	-6.17724900	-3.90692800	1.35338000
C	-2.88846800	-1.67906700	-2.30934700
H	-4.99210700	-1.49928600	-5.56575400
H	-6.43800300	-1.80170400	3.34184100
C	-6.49607000	-1.35039800	-3.09099400
H	-6.97963100	-0.59286700	-3.71833700
H	-7.04456700	-2.28960000	-3.25016800
C	-6.31338600	-3.02780600	0.71354200
C	-5.56988100	-3.15976800	-0.63537300
H	-4.64233800	-3.72553900	-0.49268100
H	-6.15894000	-3.66001900	-1.41108000
C	-3.60363300	1.79165800	2.47847400

C	-2. 62614100	1. 81263200	3. 50182900
C	-4. 06706200	3. 00726200	1. 91456800
C	-2. 12866300	0. 61855800	4. 11575700
C	-2. 09067700	3. 07721100	3. 95583300
C	-3. 52912500	4. 26418300	2. 38368900
C	-1. 17266100	0. 66680400	5. 09666900
H	-2. 51108200	-0. 33928100	3. 78542200
C	-1. 10191500	3. 08363400	4. 98987000
C	-2. 55372600	4. 26502400	3. 38462300
C	-0. 65330900	1. 91472200	5. 54584500
H	-0. 80025900	-0. 25930200	5. 52425900
H	-0. 71660500	4. 04358500	5. 32654900
H	-2. 15396500	5. 21471000	3. 73508100
H	0. 09698000	1. 93430400	6. 33220800
C	-0. 74378300	-1. 84901600	-3. 69084600
C	-0. 01252200	-0. 77904400	-4. 26247300
C	-0. 08243400	-3. 04868700	-3. 33135800
C	-0. 61931500	0. 46595500	-4. 63086100
C	1. 40683300	-0. 92579900	-4. 49452600
C	1. 34849700	-3. 15806300	-3. 51035600
C	0. 10048400	1. 45948000	-5. 24256100
H	-1. 66966100	0. 61787200	-4. 41377300
C	2. 12145500	0. 13244600	-5. 14022400
C	2. 05143700	-2. 09971400	-4. 09445100
C	1. 48748000	1. 28566700	-5. 52064800
H	-0. 38854800	2. 39002800	-5. 51758000
H	3. 18242700	-0. 00764400	-5. 33474900
H	3. 12263100	-2. 20095400	-4. 25905500
H	2. 03675600	2. 07119700	-6. 03320500
C	-5. 54410500	4. 25343300	0. 41404900
H	-6. 32873600	4. 26064200	-0. 33815000
C	-5. 09090000	3. 06019700	0. 91400900
H	-5. 52368400	2. 13144100	0. 56018800
C	-5. 00658800	5. 48771800	0. 87792200
H	-5. 38374500	6. 42511200	0. 47707200
C	-4. 02572300	5. 48675800	1. 83289100
H	-3. 60854900	6. 42136900	2. 20074600
C	-0. 10332200	-5. 32903300	-2. 45475300
H	-0. 65455500	-6. 17627700	-2. 05623100
C	1. 31189200	-5. 41209100	-2. 58317200
H	1. 83192600	-6. 31109600	-2. 26602400
C	2. 01343200	-4. 35855900	-3. 10512600
H	3. 09344100	-4. 41474200	-3. 21598500
C	-0. 77439500	-4. 18973200	-2. 81401300

H	-1. 85105200	-4. 14114200	-2. 70032500
C	2. 18069100	3. 86682100	-1. 25119300
C	2. 97930200	4. 10693700	0. 07488400
H	4. 02247900	3. 88918300	-0. 16191900
H	2. 95465600	5. 19097500	0. 25085100
C	2. 58906500	3. 43197600	1. 39220700
C	2. 19770500	2. 37855900	-1. 70457300
H	3. 20764100	2. 12638200	-2. 01809800
H	1. 57465000	2. 26371000	-2. 59570400
N	1. 75688400	1. 33838300	-0. 76393400
C	2. 51110800	0. 42150600	-0. 17924100
N	1. 95742200	-0. 57430800	0. 51774000
C	2. 71949900	-1. 62473200	1. 12878500
C	2. 93613900	-1. 60140200	2. 50704600
C	3. 21774800	-2. 66561700	0. 34572000
C	3. 69609200	-2. 61038800	3. 09451800
C	3. 97441000	-3. 67392000	0. 94755400
H	3. 00735300	-2. 69047600	-0. 71797400
C	4. 22201600	-3. 64591500	2. 31908500
H	4. 82600100	-4. 41842000	2. 77997800
C	4. 48269500	-4. 81760000	0. 10744200
C	3. 92812600	-2. 59486400	4. 58472900
F	5. 55028900	-5. 41919700	0. 67231700
F	4. 85642500	-4. 39916300	-1. 12504700
F	3. 53804600	-5. 76709000	-0. 07113500
F	3. 95233600	-1. 33161700	5. 06642800
F	5. 10679500	-3. 17515400	4. 90531500
F	2. 96408900	-3. 25876100	5. 25032300
S	4. 29080800	0. 37677400	-0. 27271600
H	2. 51308000	-0. 80285500	3. 10327800
H	0. 91696000	-0. 60949700	0. 64840400
H	0. 73572600	1. 12480100	-0. 77383200
C	3. 52500100	2. 97834900	2. 26119600
H	4. 44674300	1. 67174400	-0. 59724900
N	-0. 87847200	-0. 90025800	0. 94149000
S	-1. 12889800	-2. 12118000	1. 95925800
O	-2. 52017400	-2. 32056800	2. 38105900
O	-0. 06654600	-2. 06463500	2. 97266800
C	-0. 72630900	-3. 68914000	0. 99603200
F	0. 29484000	-3. 46766800	0. 15142700
F	-1. 78082800	-4. 12157500	0. 29810500
F	-0. 36698100	-4. 64624200	1. 85764000
C	0. 76269300	4. 47833600	-1. 21432300
C	0. 60453100	5. 83180300	-0. 86191800

C	-0.39226200	3.77151100	-1.57552700
C	-0.64505900	6.44719100	-0.86249400
H	1.46789800	6.42640600	-0.57625000
C	-1.65003500	4.38172700	-1.56295300
H	-0.35942500	2.72400300	-1.84617800
C	-1.78526500	5.72174700	-1.21164200
H	-0.72579700	7.49492400	-0.58354000
H	-2.52500700	3.78902800	-1.81347300
H	-2.76472000	6.18933100	-1.19295800
C	2.93233300	4.65941400	-2.41476700
H	2.32158500	4.53064600	-3.31759100
H	2.85275200	5.71798200	-2.16278800
C	4.37690300	4.31474000	-2.75878700
C	5.44303200	4.98983700	-2.27099900
C	1.11567500	3.47375000	1.73465300
H	0.74008500	4.50116500	1.65447300
H	0.50645900	2.88290100	1.04332300
H	0.89558800	3.12670900	2.74307700
C	4.57504800	3.22311900	-3.80879000
H	5.12599000	2.35118900	-3.43027700
H	3.61862400	2.85413200	-4.18690900
H	5.13866500	3.59606600	-4.67260900
C	3.20630600	2.36185900	3.61016200
H	3.50831900	3.03550100	4.42569800
H	2.15472700	2.11565700	3.75959100
H	3.78546800	1.43887000	3.75265100
C	6.86541300	4.66152600	-2.67348800
H	7.51889700	4.63521500	-1.79125300
H	6.96727600	3.70641700	-3.19193100
H	7.27175200	5.44324000	-3.33204600
C	5.37681200	6.16482600	-1.32181100
H	5.98709000	6.99224300	-1.70908700
H	4.36877900	6.54596400	-1.15338400
H	5.79945800	5.90530300	-0.34091300
C	5.02614400	3.07969700	2.06976400
H	5.49897200	2.09071100	2.14106100
H	5.34529300	3.53942200	1.13246100
H	5.45827700	3.68179600	2.88201300

INT-16' -4

0 imaginary frequency

H = -5472.486565

G = -5472.704679

E(M06-2X-DCM) = -5473.466307

O	-1.28368700	1.51297500	1.22771100
O	-3.30483600	-0.11348200	0.98509800
P	-1.68462000	-0.00580900	0.71335200
O	-1.01578500	-1.09499900	1.46566600
C	-2.32279600	2.63259600	5.13944800
C	-3.22108900	2.78278700	4.09008000
C	-2.86039700	2.44522700	2.77620000
C	-0.65890000	1.76502100	3.56894200
C	-1.04858100	2.14454000	4.86531900
C	-4.23077800	0.65328400	0.28121900
C	-4.35255600	2.01338400	0.56656200
C	-5.08771400	2.83916400	-0.29500000
C	-5.85407100	2.28191000	-1.31354900
C	-5.89065700	0.89377100	-1.44490800
C	-5.07304200	0.04334000	-0.67582700
H	-0.32495500	2.04029600	5.66856200
H	-6.55521800	0.44272600	-2.17518200
C	-3.98426300	2.81054200	1.81371200
C	-5.20925000	2.78418900	2.79856000
H	-5.55460300	1.74884700	2.90003300
H	-6.05026100	3.37922200	2.43092600
H	-5.87320600	4.71216600	0.48150400
H	-4.63070200	4.92049300	-0.74670900
C	-1.60018100	1.89652200	2.52885300
H	-2.60467000	2.89132400	6.15693500
H	-6.45066700	2.90838200	-1.97216900
C	-4.64906800	3.27189800	4.14653800
H	-5.19943000	2.87448900	5.00699200
H	-4.68806700	4.36790600	4.22430800
C	-4.93106200	4.29381200	0.10135900
C	-3.84365300	4.24081800	1.20342400
H	-2.85067100	4.34311500	0.75553300
H	-3.95608100	5.02817100	1.95610700
C	-5.19399200	-1.44002900	-0.83769600
C	-5.02154300	-2.04315800	-2.11117200
C	-5.58244300	-2.23882700	0.27228500
C	-4.65152900	-1.30710600	-3.28197800
C	-5.20674000	-3.46858500	-2.26240500
C	-5.73889400	-3.66645700	0.10753000
C	-4.50215400	-1.91659400	-4.49981000
H	-4.46418700	-0.24646200	-3.19207900
C	-5.04198500	-4.06782100	-3.55053300
C	-5.54424500	-4.24093400	-1.15028400
C	-4.70676300	-3.31736700	-4.64366100

H	-4.20840100	-1.32581900	-5.36354900
H	-5.18996100	-5.14182100	-3.63779100
H	-5.67031700	-5.31550700	-1.26823400
H	-4.58432400	-3.78507000	-5.61700700
C	0.76664700	1.32053100	3.41878200
C	1.16617700	0.05283400	3.90265200
C	1.73997200	2.26333500	3.00585700
C	0.22359700	-0.94099700	4.32105300
C	2.57367000	-0.26308300	4.00740800
C	3.14457500	1.94569800	3.13429800
C	0.63835200	-2.14753600	4.81915500
H	-0.83291600	-0.73471100	4.20831900
C	2.96352200	-1.53399800	4.53607700
C	3.52253700	0.69322700	3.63013400
C	2.02562300	-2.44796300	4.93632200
H	-0.09639400	-2.88925700	5.11890400
H	4.02503700	-1.75185000	4.62666400
H	4.58096300	0.47116900	3.76368200
H	2.33465900	-3.40681400	5.34409700
C	-6.25218800	-2.49813700	2.61344600
H	-6.47201300	-2.05120000	3.57952400
C	-5.87851200	-1.69843000	1.56519700
H	-5.81976400	-0.62708500	1.71252000
C	-6.36163300	-3.90765500	2.45245800
H	-6.65129800	-4.52788600	3.29659700
C	-6.11617600	-4.46916800	1.22946000
H	-6.21291800	-5.54236700	1.08104600
C	2.35557200	4.46999300	2.15292700
H	2.05929400	5.43748100	1.75855700
C	3.73706300	4.16233800	2.30585000
H	4.48674800	4.90463300	2.04497200
C	4.11540100	2.93542200	2.78163400
H	5.16859000	2.69284000	2.90947800
C	1.39358700	3.55633600	2.49795200
H	0.34669500	3.80864100	2.37892000
C	3.74317000	-3.73482200	-0.45339400
C	4.00857800	-3.93781700	-1.99582200
H	5.03574500	-3.60652300	-2.17254500
H	4.02487300	-5.02319000	-2.16080900
C	3.08297500	-3.33365200	-3.04334600
C	3.95727500	-2.25815500	-0.04793300
H	4.97995300	-1.97918700	-0.31750500
H	3.86524500	-2.16922900	1.04109900
N	3.05406100	-1.28908700	-0.68688300

C	3.26866100	0.01119500	-0.82220100
N	2.39483400	0.74851900	-1.52016300
C	2.34235400	2.16401600	-1.66017100
C	3.42082700	2.88165400	-2.18052500
C	1.14716100	2.81405500	-1.33215800
C	3.31896000	4.26497600	-2.33065200
C	1.05541400	4.19394100	-1.51234400
H	0.30729200	2.24662300	-0.94031500
C	2.13759400	4.92693500	-2.00143800
H	2.05753500	5.99932100	-2.13365300
C	-0.21428300	4.91145600	-1.12386300
C	4.46507600	5.03373600	-2.93693700
F	-0.22142900	5.23966100	0.19336600
F	-1.30441500	4.15459500	-1.34589100
F	-0.36291600	6.06438900	-1.81150600
F	5.65290200	4.44792700	-2.66912700
F	4.51639800	6.29896800	-2.47090900
F	4.35513900	5.10904100	-4.28157500
S	4.69673200	0.80219400	-0.13233600
H	4.32645600	2.37137300	-2.48920100
H	1.56070100	0.21386600	-1.83884800
H	2.15425900	-1.62657700	-1.04773500
C	3.43838200	-2.29330000	-3.83118000
H	4.75363800	-0.00164400	0.94810000
N	-1.38973300	0.22953600	-0.87747800
S	-0.97130900	-0.88173500	-1.90227700
O	-1.79166800	-2.08625700	-2.01553200
O	0.51629200	-1.13806600	-1.93954800
C	-1.15422300	0.09719500	-3.48855300
F	-0.17176900	1.01784600	-3.57079700
F	-2.32335100	0.72930600	-3.57261500
F	-1.03348100	-0.73699500	-4.52820600
C	2.37896600	-4.29729700	-0.01506000
C	2.07039700	-5.64275100	-0.28957700
C	1.41511300	-3.54418100	0.67010900
C	0.85441300	-6.20252000	0.09329800
H	2.78635900	-6.26865000	-0.81555200
C	0.18434500	-4.09532700	1.04336100
H	1.58229500	-2.50541200	0.93327800
C	-0.09947300	-5.42753900	0.75769500
H	0.64895000	-7.24490400	-0.13740000
H	-0.53960400	-3.45319000	1.53364300
H	-1.05649700	-5.85732000	1.04006700
C	4.91873800	-4.52958300	0.25229600

H	4.74286100	-5.59121900	0.04347900
H	5.83663400	-4.27256500	-0.28218000
C	5.12294500	-4.36961300	1.75131600
C	6.15915300	-3.67901700	2.28128100
C	1.76049900	-4.04849600	-3.24502200
H	1.00803600	-3.74900500	-2.50717900
H	1.33564400	-3.85608900	-4.23254500
H	1.88888600	-5.13228100	-3.14412300
C	4.11066300	-5.10143100	2.61849200
H	3.70017600	-5.96418600	2.08621200
H	4.54758700	-5.46941500	3.55046300
H	3.25513000	-4.46584700	2.87848000
C	2.52144900	-1.76917100	-4.92677700
H	2.91046000	-0.83473800	-5.34577900
H	2.43743500	-2.48060400	-5.75979800
H	1.50879400	-1.57163800	-4.56457900
C	6.39470500	-3.54536200	3.77169500
H	7.31287900	-4.07274100	4.06920700
H	6.55090700	-2.49131300	4.04137200
H	5.57691100	-3.92281000	4.38616400
C	4.74954600	-1.54358600	-3.75741400
H	4.57274700	-0.47912300	-3.54392800
H	5.45043900	-1.91625700	-3.00785800
H	5.25947400	-1.57218200	-4.73077200
C	7.23491400	-2.96200600	1.49202100
H	7.18280000	-3.10476600	0.41149800
H	7.20430500	-1.87928600	1.68535800
H	8.22952500	-3.29560300	1.81941100

INT-16' -5

0 imaginary frequency

H = -5472.499956

G = -5472.718673

E(M06-2X-DCM) = -5473.479546

O	1.82553800	-2.70954600	-0.23661400
O	3.32125100	-0.59758500	-0.08394200
P	1.77029600	-1.09605000	0.08065200
O	1.32986800	-0.76459300	1.45884400
C	3.97025700	-4.91938400	2.59957400
C	4.61575300	-4.33823100	1.51313100
C	3.88344200	-3.66452100	0.52463600
C	1.82184200	-4.10775400	1.75271400
C	2.58133600	-4.82365000	2.69293900
C	4.03932400	-0.79890700	-1.25638000

C	4. 59015400	-2. 05248600	-1. 52541200
C	5. 17350500	-2. 28633300	-2. 78057600
C	5. 32146900	-1. 25282000	-3. 69964200
C	4. 89055100	0. 02752800	-3. 35296700
C	4. 23391600	0. 28429200	-2. 13749000
H	2. 06152500	-5. 29340100	3. 52306500
H	5. 04530500	0. 85425700	-4. 04004900
C	4. 79587100	-3. 27520600	-0. 63243000
C	6. 16859400	-3. 18730900	0. 12004600
H	6. 24357100	-2. 20375700	0. 59808100
H	7. 02342400	-3. 29639300	-0. 55475100
H	6. 66269200	-3. 86231400	-2. 86122100
H	5. 26087000	-4. 16808400	-3. 88069000
C	2. 50922100	-3. 50224700	0. 68374700
H	4. 53415200	-5. 44378200	3. 36708500
H	5. 78225800	-1. 43060000	-4. 66818800
C	6. 09592300	-4. 28501600	1. 20366200
H	6. 70275700	-4. 04936600	2. 08546400
H	6. 45815400	-5. 24968700	0. 82056300
C	5. 57197000	-3. 74006600	-2. 92066500
C	4. 86416500	-4. 40083000	-1. 71731300
H	3. 84211600	-4. 68155500	-1. 99627200
H	5. 37131100	-5. 30055500	-1. 35451200
C	3. 83119400	1. 68742200	-1. 80597700
C	2. 89322300	2. 36976200	-2. 62000000
C	4. 46714500	2. 36930700	-0. 73643400
C	2. 18914800	1. 73130900	-3. 69100000
C	2. 60662000	3. 76480200	-2. 37062800
C	4. 14189400	3. 75393000	-0. 47656500
C	1. 31304900	2. 42513300	-4. 48400500
H	2. 33681200	0. 67157100	-3. 85247800
C	1. 69077500	4. 45483300	-3. 22593400
C	3. 22880700	4. 41534600	-1. 30236200
C	1. 07072800	3. 81091100	-4. 26258900
H	0. 78484200	1. 90864100	-5. 28047400
H	1. 50366600	5. 50899900	-3. 03329200
H	2. 99422500	5. 45971900	-1. 10802100
H	0. 38353200	4. 34825000	-4. 91084000
C	0. 33275700	-4. 05879800	1. 90303600
C	-0. 25253500	-3. 33459800	2. 96877300
C	-0. 48013200	-4. 82149800	1. 02963800
C	0. 51288600	-2. 51633700	3. 86126000
C	-1. 68206600	-3. 39638200	3. 17410400
C	-1. 90968600	-4. 85996200	1. 23606200

C	-0.08100800	-1.83921600	4.89380900
H	1.57564100	-2.40839200	3.68628100
C	-2.26118900	-2.68090400	4.26923700
C	-2.46983300	-4.15363100	2.30363700
C	-1.48614100	-1.92925800	5.11041700
H	0.52347100	-1.21163200	5.54264100
H	-3.33688800	-2.75020300	4.41683000
H	-3.54573700	-4.19866200	2.46318800
H	-1.93869200	-1.39208400	5.94039000
C	6.04129100	2.44068500	1.13500300
H	6.78204600	1.94535900	1.75677900
C	5.45306300	1.75755600	0.10316500
H	5.73933800	0.73035300	-0.08801600
C	5.69481200	3.79511300	1.40267300
H	6.17064000	4.32061300	2.22656600
C	4.77548800	4.43146400	0.61290700
H	4.50305400	5.46709200	0.80019700
C	-0.75789900	-6.33041000	-0.87440400
H	-0.32362200	-6.90550600	-1.68794800
C	-2.16741000	-6.35371800	-0.67439400
H	-2.79597800	-6.94544400	-1.33486300
C	-2.72198400	-5.64036400	0.35446200
H	-3.79610700	-5.65698700	0.52546100
C	0.05347500	-5.59447500	-0.05108300
H	1.12523200	-5.59490900	-0.21386500
N	0.98944200	-0.46974400	-1.21100100
S	-0.51507200	-0.74850800	-1.54126900
O	-1.25067500	0.54693100	-1.77709000
O	-1.23705600	-1.72544800	-0.71005600
C	-0.48137400	-1.48739000	-3.25623400
F	0.13255400	-0.67514700	-4.12532400
F	-1.73984900	-1.68496600	-3.67422600
F	0.15765600	-2.65769300	-3.23003200
C	-5.73456400	0.75368100	-0.83155700
C	-5.74773000	1.94023900	-1.86895300
H	-6.08756900	2.82324200	-1.32064700
H	-6.55080000	1.71705700	-2.58363400
C	-4.49500100	2.27276600	-2.66612900
C	-4.79479600	1.06407400	0.35799800
H	-5.17721900	1.97069700	0.83704700
H	-4.86013400	0.25634600	1.09427100
N	-3.37717300	1.30831100	0.04168500
C	-2.53801700	1.94966900	0.84059200
N	-1.26315300	2.13526200	0.47813000

C	-0.24725100	2.80059700	1.24489500
C	-0.03852800	4.16843000	1.05387000
C	0.56019100	2.06463700	2.11680300
C	0.97882500	4.81013800	1.76075700
C	1.57254500	2.72471400	2.81711800
H	0.44264200	0.98773300	2.20271200
C	1.78208200	4.09291000	2.64809000
H	2.57664200	4.59131700	3.18874100
C	2.48439000	1.92734600	3.72226400
C	1.17359200	6.29302900	1.58204300
F	1.79614600	0.98916100	4.40580200
F	3.45319300	1.30574300	3.03316700
F	3.08720600	2.72951300	4.63418000
F	0.29520700	7.00285900	2.32648300
F	2.41232300	6.68996200	1.94367900
F	0.98533000	6.66640800	0.29515500
S	-3.17090000	2.55406600	2.38000200
H	-0.65114500	4.71612800	0.34557300
H	-0.98628200	1.65550100	-0.40058100
H	-2.96506800	0.91846500	-0.81299300
C	-3.75639900	3.38592500	-2.45860800
H	-1.98979200	3.06040100	2.78643700
C	-7.19004800	0.74791500	-0.20101500
H	-7.87967500	0.48775400	-1.01228500
H	-7.42178200	1.78326300	0.06312800
C	-5.45434400	-0.60060500	-1.50458000
C	-4.43143000	-1.46506600	-1.09489700
C	-6.27719800	-1.02748500	-2.56395400
C	-4.22529500	-2.69907700	-1.72198800
H	-3.75738200	-1.20488000	-0.28701000
C	-6.08485900	-2.25901400	-3.18381900
H	-7.08594200	-0.39202500	-2.91437600
C	-5.05348500	-3.10332200	-2.76490300
H	-3.40505800	-3.32579300	-1.38813800
H	-6.74064200	-2.55756900	-3.99785800
H	-4.89565900	-4.06167700	-3.25207100
C	-7.46803800	-0.17303900	0.97988600
C	-7.57031000	0.27462300	2.25292500
C	-7.68034800	-1.63192600	0.61225400
H	-6.73354100	-2.17397200	0.50046300
H	-8.28883800	-2.16753200	1.34366800
H	-8.18868200	-1.70972100	-0.35481100
C	-7.83875200	-0.62733700	3.44032800
H	-8.83346800	-0.42792200	3.86476600

H	-7.77507000	-1.69233500	3.21579500
H	-7.11711500	-0.41872200	4.24189800
C	-4.14457200	1.31932400	-3.79533600
H	-5.04358600	0.84557500	-4.20096900
H	-3.64164700	1.83533300	-4.61802600
H	-3.47964600	0.50894300	-3.47230200
C	-2.52695200	3.68402300	-3.30164700
H	-1.97172300	4.53806300	-2.90010200
H	-1.83672200	2.83501900	-3.33784600
H	-2.79355800	3.93460900	-4.33804900
C	-4.02789000	4.44101800	-1.41096200
H	-4.10702000	5.43070100	-1.88210700
H	-4.93495500	4.28271100	-0.82436900
H	-3.18742900	4.51066300	-0.70461400
C	-7.43782600	1.71985800	2.68688600
H	-7.41654900	2.44222300	1.86879500
H	-8.27673000	1.99240400	3.34177800
H	-6.52676800	1.86641600	3.28527400

INT-16' -6

0 imaginary frequency

H = -5472.500134

G = -5472.715926

E(M06-2X-DCM) = -5473.479127

O	-2.30475200	-2.60852000	0.38269200
O	-2.97757200	-0.13876200	0.68588100
P	-1.66634900	-1.11639600	0.60394400
O	-0.83587200	-0.66186800	-0.55807700
C	-5.22958400	-3.38976700	-2.51254000
C	-5.58189100	-2.90121400	-1.25916500
C	-4.60821200	-2.66791900	-0.27516200
C	-2.87574900	-3.35740400	-1.85256800
C	-3.88484200	-3.62625900	-2.79202000
C	-3.77222000	-0.19089000	1.83415300
C	-4.65822800	-1.24839700	2.01899700
C	-5.23120600	-1.44004600	3.28553800
C	-5.04502600	-0.50086300	4.29506100
C	-4.29890700	0.64876700	4.02414400
C	-3.63842600	0.82559400	2.79832900
H	-3.59291400	-4.01015800	-3.76529700
H	-4.19808900	1.42040600	4.78192900
C	-5.27002400	-2.23841900	1.03159300
C	-6.61545400	-1.65032900	0.47289300
H	-6.43756200	-0.61883500	0.14730200

H	-7.40642900	-1.62880700	1.22840800
H	-7.08451200	-2.57465900	3.36227600
H	-5.74588100	-3.35065700	4.20010800
C	-3.26398400	-2.86503600	-0.59098100
H	-5.98701500	-3.57612800	-3.26971500
H	-5.48926700	-0.64312400	5.27702300
C	-6.95407200	-2.52324300	-0.75069600
H	-7.55177600	-1.99234700	-1.50031900
H	-7.52892700	-3.41424200	-0.46016100
C	-5.99979900	-2.74601700	3.32188900
C	-5.58399600	-3.42773200	1.99498300
H	-4.66928700	-4.01177000	2.14618900
H	-6.35069100	-4.09968400	1.59549500
C	-2.89408800	2.09257800	2.50995100
C	-1.70973800	2.41771800	3.21349800
C	-3.43186800	3.00385200	1.56400400
C	-1.09722500	1.52396700	4.15007000
C	-1.05985900	3.68765600	2.97160100
C	-2.75843500	4.25863300	1.31659200
C	0.05007700	1.86759900	4.81651100
H	-1.53092900	0.54333500	4.30144500
C	0.12544100	4.01469900	3.70311200
C	-1.59452000	4.56700200	2.02693100
C	0.66348500	3.13517100	4.60448200
H	0.50732900	1.15246800	5.49283100
H	0.58613600	4.98464600	3.52748700
H	-1.09055700	5.51135300	1.83359400
H	1.56408200	3.39537000	5.15481700
C	-1.44985400	-3.60365900	-2.23303500
C	-0.83939200	-2.78941200	-3.21769100
C	-0.73954800	-4.68773800	-1.66548000
C	-1.49482600	-1.65984700	-3.80811900
C	0.50916800	-3.08011200	-3.64877700
C	0.61523900	-4.95566200	-2.09131600
C	-0.88100400	-0.89531400	-4.76712600
H	-2.49298800	-1.39918800	-3.47528200
C	1.11192400	-2.26089200	-4.65511500
C	1.19857400	-4.15121200	-3.07391100
C	0.43989400	-1.20215000	-5.20419700
H	-1.40139900	-0.03814300	-5.18556500
H	2.12291200	-2.50293900	-4.97633800
H	2.21454200	-4.36598100	-3.40081200
H	0.90910100	-0.59086300	-5.97072200
C	-5.13059500	3.64984800	-0.07557100

H	-6.04933200	3.42760300	-0.61173700
C	-4.64122300	2.75276300	0.83798500
H	-5.18146600	1.83187700	1.02406700
C	-4.45173500	4.87542200	-0.32680800
H	-4.85510600	5.57533600	-1.05384200
C	-3.30201300	5.16911000	0.35586300
H	-2.77238300	6.10101400	0.17801700
C	-0.59411400	-6.59142000	-0.14107500
H	-1.05079700	-7.23144200	0.60895400
C	0.74615800	-6.84132700	-0.55287300
H	1.29939100	-7.66653000	-0.11249500
C	1.32796200	-6.04723700	-1.50350700
H	2.34783700	-6.23269000	-1.83307100
C	-1.31082100	-5.55633900	-0.68125700
H	-2.33178500	-5.38320900	-0.36074600
N	-1.05140300	-1.23028700	2.09150900
S	0.45125600	-1.43295500	2.50004200
O	0.62104600	-1.38968100	3.95215100
O	1.42429000	-0.65150700	1.68536700
C	0.85942000	-3.19892000	2.02892300
F	0.01507200	-4.05442300	2.60274400
F	2.11208700	-3.50253700	2.42248100
F	0.79733600	-3.34353600	0.69819200
C	5.55698000	0.19156600	0.29123000
C	5.70830500	1.75664400	0.30030200
H	5.91320900	2.04565000	-0.73560100
H	6.65086900	1.96355500	0.82617600
C	4.64214700	2.68724900	0.88877100
C	4.36555700	-0.28346400	-0.59417900
H	4.62153200	-0.10259200	-1.63751000
H	4.25532100	-1.36621800	-0.49833400
N	3.03422500	0.29942400	-0.36971300
C	2.34657500	1.06644100	-1.20299500
N	1.02616600	1.20650400	-1.05348900
C	0.21756100	2.23827700	-1.61676600
C	0.55609000	3.58350800	-1.46032400
C	-0.96379100	1.87620200	-2.26758400
C	-0.26795800	4.56642000	-2.00681300
C	-1.78695700	2.87271400	-2.78945300
H	-1.22976300	0.82925500	-2.34263500
C	-1.44284700	4.21945800	-2.67464500
H	-2.08618300	4.98701500	-3.08640700
C	-3.02806800	2.47451300	-3.54588800
C	0.09113700	6.01503300	-1.80842500

F	-3.57063300	1.33904200	-3.06619400
F	-3.97330900	3.43660200	-3.50530300
F	-2.75052500	2.25248800	-4.85838300
F	-0.31445400	6.48044400	-0.60081300
F	1.43211000	6.20713300	-1.86101500
F	-0.46886000	6.80742300	-2.74372400
S	3.08212600	1.85982900	-2.61440500
H	1.45034900	3.85833900	-0.91467300
H	0.47590000	0.43336200	-0.60741200
H	2.49189000	-0.05940900	0.43204700
C	4.39302900	3.90368700	0.34574600
H	4.29281400	2.04816800	-2.06077000
C	6.84635300	-0.33074800	-0.47779900
H	7.71209200	-0.05925000	0.13748200
H	6.93229300	0.26389100	-1.39195200
C	5.56389400	-0.39349000	1.71790900
C	4.60303200	-1.29465000	2.19067500
C	6.60656000	-0.04537700	2.59727100
C	4.66304400	-1.81128400	3.48899300
H	3.76890600	-1.60349900	1.57420600
C	6.67804400	-0.56404600	3.88804500
H	7.38342900	0.64369700	2.27781800
C	5.70022200	-1.45034700	4.34406500
H	3.88093400	-2.48451100	3.82302000
H	7.49823200	-0.27073900	4.53838700
H	5.74576200	-1.84919100	5.35359700
C	6.93593500	-1.81439100	-0.80848600
C	6.72419600	-2.30676200	-2.05076000
C	7.34249700	-2.71250700	0.35010700
H	7.95418800	-2.15833200	1.06838700
H	6.47941400	-3.08851000	0.91289100
H	7.92710200	-3.57506800	0.02078400
C	6.79477100	-3.78425500	-2.37818900
H	5.91917300	-4.08033500	-2.97179700
H	7.67496100	-4.00710200	-2.99889400
H	6.82690200	-4.43134300	-1.50100600
C	4.02730500	2.26462000	2.20655300
H	3.37574600	3.02738100	2.63171500
H	3.44106200	1.34381700	2.13297900
H	4.81538500	2.06088800	2.94141700
C	3.41626900	4.90301400	0.94471000
H	2.96523400	5.51633300	0.15555300
H	2.60204800	4.44464100	1.50980600
H	3.93275500	5.60205500	1.61886500

C	5.10266700	4.49969400	-0.85500300
H	5.58638000	5.44187600	-0.56041400
H	5.88264400	3.87428100	-1.29470100
H	4.38724700	4.76520300	-1.64591000
C	6.39688000	-1.48577700	-3.28055100
H	5.36035600	-1.65693600	-3.60580500
H	6.53169800	-0.40905900	-3.15755800
H	7.03379600	-1.79912700	-4.11886100

INT-16' -7

0 imaginary frequency

H = -5472.496578

G = -5472.712461

E(M06-2X-DCM) = -5473.478182

O	2.25198100	-2.56037100	0.58662100
O	3.62055000	-0.52817700	-0.22434700
P	2.08544400	-1.06219000	-0.07524700
O	1.35773200	-0.11942800	0.83152200
C	4.17918700	-2.96378900	4.29303400
C	4.90889700	-2.90928500	3.11153500
C	4.26107600	-2.83384600	1.86830700
C	2.10599000	-2.75153700	3.00707600
C	2.78980100	-2.90830300	4.22666900
C	4.53214200	-1.16869000	-1.06681400
C	5.16436700	-2.33493700	-0.63525900
C	5.94436600	-3.06898900	-1.54290400
C	6.22091400	-2.56496100	-2.80824600
C	5.69596300	-1.32572100	-3.16880500
C	4.81886700	-0.61340200	-2.33112000
H	2.20489600	-2.95680000	5.14024200
H	5.93601400	-0.90163600	-4.13877500
C	5.28614300	-2.96958000	0.74749000
C	6.56295000	-2.42421100	1.47710700
H	6.54695400	-1.32882400	1.43993400
H	7.49019200	-2.75947200	1.00326200
H	7.45488200	-4.38221600	-0.69623700
H	6.21170200	-5.23028000	-1.60833800
C	2.87169300	-2.70638500	1.82383000
H	4.67927300	-3.04030200	5.25520700
H	6.84433800	-3.11879200	-3.50579200
C	6.41036900	-2.89634000	2.93635400
H	6.91043700	-2.23481800	3.65299000
H	6.83786600	-3.89865000	3.08079900
C	6.38170900	-4.38372700	-0.93311200

C	5. 52060600	-4. 46306100	0. 34684600
H	4. 55236200	-4. 92220000	0. 11716500
H	5. 98588900	-5. 04455300	1. 14908000
C	4. 26120900	0. 68679000	-2. 81393300
C	3. 53925200	0. 72625500	-4. 03593800
C	4. 53869800	1. 89047300	-2. 11559400
C	3. 19437400	-0. 44970700	-4. 78002300
C	3. 11438400	1. 99906100	-4. 57432500
C	4. 05626700	3. 14835400	-2. 63987700
C	2. 54986900	-0. 36955000	-5. 98669900
H	3. 42730400	-1. 42121600	-4. 36253400
C	2. 44172400	2. 03838600	-5. 83605600
C	3. 36986100	3. 16952700	-3. 85632700
C	2. 17968400	0. 89118300	-6. 53396600
H	2. 29661400	-1. 28064100	-6. 52185600
H	2. 14369200	3. 00825300	-6. 22808200
H	3. 03393500	4. 12319900	-4. 25925800
H	1. 67136200	0. 93482900	-7. 49358700
C	0. 61563600	-2. 63812100	3. 06832900
C	0. 04447700	-1. 56851700	3. 80458400
C	-0. 21762600	-3. 64926200	2. 53006200
C	0. 81908500	-0. 47080500	4. 30515100
C	-1. 37603400	-1. 55669600	4. 07021000
C	-1. 64490800	-3. 59701700	2. 75904200
C	0. 25301200	0. 52589900	5. 05799200
H	1. 87419500	-0. 42568300	4. 06400800
C	-1. 92460400	-0. 51520700	4. 88474800
C	-2. 18193500	-2. 56791700	3. 53885200
C	-1. 13629100	0. 49399000	5. 37420100
H	0. 86725000	1. 35216900	5. 40423000
H	-2. 98842900	-0. 54663300	5. 11001300
H	-3. 24997700	-2. 56337000	3. 74952800
H	-1. 56407900	1. 26913800	6. 00560800
C	5. 54230100	3. 11409400	-0. 24981200
H	6. 12424100	3. 11294200	0. 66768100
C	5. 31273200	1. 93665300	-0. 91139500
H	5. 72777700	1. 01643200	-0. 51869800
C	5. 02593700	4. 34318300	-0. 74905900
H	5. 21111900	5. 26574700	-0. 20556900
C	4. 31351900	4. 35558900	-1. 91683700
H	3. 92971700	5. 28831500	-2. 32420500
C	-0. 53882600	-5. 72246300	1. 27769800
H	-0. 12335500	-6. 54872100	0. 70777000
C	-1. 94536300	-5. 65348000	1. 48617800

H	-2.58895300	-6.42594100	1.07420700
C	-2.47831900	-4.62331600	2.21250100
H	-3.54915400	-4.57009900	2.39722900
C	0.29344000	-4.76077600	1.78706200
H	1.36133600	-4.83379800	1.62209500
N	1.56999400	-1.37346300	-1.57912600
S	0.05268600	-1.45448700	-1.98511800
O	-0.88334900	-1.44388800	-0.81685800
O	-0.20493300	-2.43741300	-3.03836700
C	-0.31662100	0.20134800	-2.77574000
F	-1.64623400	0.30619200	-2.96678400
F	0.29141800	0.34114700	-3.94731800
F	0.06466100	1.19913100	-1.95873300
C	-5.31435100	-0.72828400	-0.24400500
C	-6.00974300	0.67196700	-0.19327500
H	-6.40394200	0.76439400	0.81967300
H	-6.89766600	0.61364000	-0.83347200
C	-5.27109700	1.96085300	-0.56151700
C	-4.09653000	-0.77614400	0.73287800
H	-4.43945100	-0.43871300	1.71153500
H	-3.76409600	-1.81210800	0.84963100
N	-2.88043000	-0.01087900	0.40883500
C	-2.32463100	0.94808400	1.13034500
N	-1.02665800	1.25416100	0.97290900
C	-0.44596600	2.52105100	1.27295500
C	0.73993800	2.57608100	2.01055000
C	-1.03226700	3.69377400	0.79321200
C	1.30190700	3.81817200	2.30456900
C	-0.46395000	4.92815100	1.10574500
H	-1.92248900	3.64490200	0.17734500
C	0.70165200	5.00015600	1.86735100
H	1.13837000	5.96098700	2.11088600
C	-1.16280100	6.18072000	0.64641000
C	2.59107800	3.88158500	3.08448600
F	-1.62658100	6.05714800	-0.61684600
F	-2.23691600	6.45757900	1.42783800
F	-0.35540400	7.25872400	0.68516300
F	2.70181200	2.84687100	3.94984100
F	3.67144900	3.84223200	2.27873900
F	2.67600200	5.02228200	3.80623600
S	-3.31090000	1.83265200	2.32166300
H	1.20785900	1.65586300	2.33375300
H	-0.34617100	0.51976300	0.68576100
H	-2.24821100	-0.44750000	-0.28426100

C	-5.45502500	3.10465200	0.14577200
H	-2.32180200	1.84338800	3.24407600
C	-6.29612900	-1.78515100	0.43724500
H	-6.40883200	-1.48311500	1.48906900
H	-5.75644300	-2.73601100	0.45188000
C	-4.99930700	-1.22965200	-1.66335300
C	-3.88383200	-2.03481200	-1.93818200
C	-5.88543600	-0.97848000	-2.72667600
C	-3.63772900	-2.53565700	-3.21968100
H	-3.16449200	-2.28421500	-1.16707000
C	-5.65318600	-1.48627900	-4.00414500
H	-6.77566500	-0.38093700	-2.56762300
C	-4.52275300	-2.26420300	-4.26027500
H	-2.73614900	-3.11454600	-3.39290300
H	-6.35785000	-1.26520500	-4.80214900
H	-4.33221100	-2.64733300	-5.25911500
C	-7.68773400	-1.99114700	-0.13657300
C	-7.99880200	-3.01051600	-0.96786000
C	-8.75796500	-1.01961800	0.35137400
H	-9.06413100	-0.29679300	-0.41684300
H	-9.66474300	-1.54026100	0.67732700
H	-8.40184000	-0.43880600	1.20733900
C	-9.39387100	-3.21677800	-1.51734000
H	-9.36133300	-3.28298200	-2.61353100
H	-9.81312500	-4.17057700	-1.16575200
H	-10.09638600	-2.42373500	-1.25637900
C	-4.49248600	1.92458500	-1.85971100
H	-3.99153800	2.86568300	-2.08740400
H	-3.73534900	1.13730000	-1.86994100
H	-5.16263400	1.70146500	-2.69965800
C	-4.85600900	4.44855000	-0.22071900
H	-4.32969600	4.88258400	0.63971000
H	-4.15632900	4.43067000	-1.05663100
H	-5.65256100	5.16111400	-0.47917500
C	-6.34285300	3.24958400	1.36623500
H	-7.19837800	3.89802600	1.12863100
H	-6.74542800	2.31751900	1.76416300
H	-5.79726200	3.74918100	2.17806900
C	-7.03632000	-4.06472500	-1.46261000
H	-6.04622900	-4.02064000	-1.00856000
H	-7.45120500	-5.06651800	-1.28273900
H	-6.89295800	-3.97316800	-2.54720400

0 imaginary frequency

H = -5472.496581

G = -5472.712463

E(M06-2X-DCM) = -5473.478192

O	2.25175400	-2.56078500	0.58550600
O	3.62056100	-0.52826000	-0.22425700
P	2.08543900	-1.06214900	-0.07542000
O	1.35790700	-0.11984600	0.83196100
C	4.17823600	-2.96635700	4.29204500
C	4.90816800	-2.91134300	3.11069600
C	4.26056000	-2.83518300	1.86741400
C	2.10527700	-2.75321900	3.00583200
C	2.78887200	-2.91068200	4.22546800
C	4.53225100	-1.16847000	-1.06684400
C	5.16428700	-2.33498700	-0.63575800
C	5.94440700	-3.06861200	-1.54365600
C	6.22127400	-2.56393100	-2.80866400
C	5.69647100	-1.32447100	-3.16869700
C	4.81923900	-0.61255300	-2.33082200
H	2.20380500	-2.95957100	5.13891600
H	5.93675000	-0.89989600	-4.13839600
C	5.28578200	-2.97039800	0.74667700
C	6.56251800	-2.42551200	1.47679500
H	6.54659200	-1.33010300	1.44022900
H	7.48981400	-2.76056900	1.00290900
H	7.45466300	-4.38251100	-0.69751600
H	6.21145900	-5.22988100	-1.61023200
C	2.87119200	-2.70754700	1.82275300
H	4.67814200	-3.04343400	5.25426700
H	6.84481500	-3.11744200	-3.50636000
C	6.40966900	-2.89844800	2.93575700
H	6.90971200	-2.23741000	3.65285400
H	6.83703200	-3.90089400	3.07966800
C	6.38151900	-4.38373000	-0.93451000
C	5.52021100	-4.46367100	0.34527100
H	4.55197800	-4.92264000	0.11520300
H	5.98533000	-5.04561300	1.14727400
C	4.26165400	0.68787500	-2.81309100
C	3.53979200	0.72790700	-4.03513500
C	4.53910600	1.89123400	-2.11418500
C	3.19495500	-0.44770400	-4.77980100
C	3.11499000	2.00097200	-4.57297300
C	4.05674800	3.14936300	-2.63792800
C	2.55054800	-0.36697700	-5.98648900

H	3. 42785700	-1. 41940900	-4. 36275600
C	2. 44242300	2. 04089100	-5. 83473900
C	3. 37043900	3. 17110400	-3. 85442700
C	2. 18041700	0. 89401800	-6. 53320000
H	2. 29732400	-1. 27781500	-6. 52209200
H	2. 14443800	3. 01094600	-6. 22633600
H	3. 03458900	4. 12497200	-4. 25695700
H	1. 67217300	0. 93811400	-7. 49284200
C	0. 61491800	-2. 63968700	3. 06689900
C	0. 04374500	-1. 57044500	3. 80368100
C	-0. 21835800	-3. 65041300	2. 52789100
C	0. 81837300	-0. 47305700	4. 30492900
C	-1. 37679500	-1. 55866700	4. 06913600
C	-1. 64566700	-3. 59819000	2. 75672600
C	0. 25225700	0. 52332200	5. 05817400
H	1. 87352300	-0. 42791500	4. 06396800
C	-1. 92540600	-0. 51755500	4. 88412500
C	-2. 18270400	-2. 56953900	3. 53711400
C	-1. 13709300	0. 49135100	5. 37416700
H	0. 86648200	1. 34939400	5. 40490900
H	-2. 98926300	-0. 54902000	5. 10923100
H	-3. 25076400	-2. 56505300	3. 74769500
H	-1. 56492700	1. 26623800	6. 00586400
C	5. 54259200	3. 11395600	-0. 24775700
H	6. 12445800	3. 11236000	0. 66978100
C	5. 31304400	1. 93682700	-0. 90990600
H	5. 72803800	1. 01641200	-0. 51760800
C	5. 02629000	4. 34328400	-0. 74647100
H	5. 21144400	5. 26559300	-0. 20253600
C	4. 31396900	4. 35625300	-1. 91430500
H	3. 93023300	5. 28918300	-2. 32127100
C	-0. 53959700	-5. 72273000	1. 27406700
H	-0. 12413800	-6. 54863200	0. 70361500
C	-1. 94616000	-5. 65375300	1. 48240900
H	-2. 58977000	-6. 42586700	1. 06981800
C	-2. 47910700	-4. 62404900	2. 20938700
H	-3. 54995800	-4. 57086300	2. 39402900
C	0. 29269600	-4. 76148900	1. 78421600
H	1. 36060700	-4. 83450600	1. 61934300
N	1. 56993200	-1. 37239100	-1. 57950400
S	0. 05263300	-1. 45352900	-1. 98546500
O	-0. 88338400	-1. 44334000	-0. 81716900
O	-0. 20494900	-2. 43623800	-3. 03895100
C	-0. 31681300	0. 20240300	-2. 77574300

F	0.06358700	1.20007200	-1.95809400
F	-1.64629800	0.30683700	-2.96761300
F	0.29199900	0.34283500	-3.94682700
C	-5.31436700	-0.72772200	-0.24399800
C	-6.00952200	0.67267100	-0.19334800
H	-6.40412700	0.76503200	0.81945100
H	-6.89722900	0.61459100	-0.83387400
C	-5.27054900	1.96147300	-0.56112700
C	-4.09678500	-0.77587700	0.73313400
H	-4.43982000	-0.43829700	1.71170300
H	-3.76469400	-1.81193200	0.85003000
N	-2.88038500	-0.01101100	0.40924500
C	-2.32445800	0.94784900	1.13081600
N	-1.02639900	1.25363000	0.97358600
C	-0.44559800	2.52045900	1.27374000
C	0.73993700	2.57543400	2.01189900
C	-1.03155600	3.69319800	0.79358800
C	1.30188900	3.81751500	2.30608400
C	-0.46331100	4.92754200	1.10631900
H	-1.92147200	3.64432400	0.17727600
C	0.70193300	4.99950400	1.86850300
H	1.13862400	5.96031200	2.11216700
C	-1.16189600	6.18016900	0.64675500
C	2.59074400	3.88074700	3.08654200
F	-2.23573900	6.45758400	1.42837000
F	-0.35415900	7.25795200	0.68502900
F	-1.62599600	6.05640100	-0.61635800
F	2.67640700	5.02220300	3.80696100
F	2.70007700	2.84693700	3.95321200
F	3.67145600	3.83933100	2.28137900
S	-3.31064500	1.83267100	2.32197700
H	1.20757600	1.65520200	2.33548700
H	-0.34597300	0.51922100	0.68628500
H	-2.24802600	-0.44796800	-0.28355600
C	-5.45428800	3.10514800	0.14640500
H	-2.32161400	1.84333400	3.24444200
C	-6.29653600	-1.78443900	0.43696900
H	-6.40937600	-1.48248500	1.48880500
H	-5.75706600	-2.73542300	0.45159900
C	-4.99910200	-1.22907500	-1.66331000
C	-3.88381400	-2.03458100	-1.93789100
C	-5.88481700	-0.97750700	-2.72688700
C	-3.63744700	-2.53533100	-3.21937900
H	-3.16484000	-2.28437200	-1.16656200

C	-5.65233000	-1.48523200	-4.00434000
H	-6.77490200	-0.37969100	-2.56805400
C	-4.52205200	-2.26346300	-4.26022000
H	-2.73598500	-3.11446900	-3.39238300
H	-6.35668300	-1.26385100	-4.80253400
H	-4.33130600	-2.64650900	-5.25905300
C	-7.68805200	-1.99004700	-0.13715100
C	-7.99920500	-3.00926400	-0.96859000
C	-8.75820600	-1.01834200	0.35065200
H	-9.06508500	-0.29632400	-0.41803400
H	-9.66463200	-1.53896600	0.67766900
H	-8.40172100	-0.43666000	1.20586100
C	-9.39426000	-3.21516700	-1.51823900
H	-9.36172000	-3.28086500	-2.61446300
H	-9.81356900	-4.16911200	-1.16710900
H	-10.09674100	-2.42222400	-1.25689200
C	-4.49176900	1.92530600	-1.85923200
H	-3.98997700	2.86609900	-2.08631800
H	-3.73526300	1.13742200	-1.86970700
H	-5.16194300	1.70317000	-2.69942800
C	-4.85527500	4.44905900	-0.22000000
H	-5.65187600	5.16164300	-0.47828300
H	-4.32881800	4.88302800	0.64036900
H	-4.15576600	4.43125500	-1.05605500
C	-6.34204700	3.24989500	1.36694600
H	-7.19834500	3.89726600	1.12918100
H	-6.74347500	2.31761800	1.76554600
H	-5.79679000	3.75054500	2.17834700
C	-7.03684400	-4.06355900	-1.46336700
H	-6.89316500	-3.97172100	-2.54789900
H	-6.04686200	-4.01981800	-1.00903500
H	-7.45198900	-5.06531500	-1.28389400

INT-16' -9

0 imaginary frequency

H = -5472.499550

G = -5472.714171

E(M06-2X-DCM) = -5473.477375

O	0.74096700	3.02045100	0.35825900
O	2.79611800	1.49359200	0.03283500
P	1.17515100	1.43318000	0.28444200
O	0.54126300	0.68991600	-0.83404900
C	1.73338700	5.45645000	-2.90550900
C	2.62273400	5.27703500	-1.85177000

C	2. 27290200	4. 49492900	-0. 74070800
C	0. 11433400	4. 01633200	-1. 76974500
C	0. 48501800	4. 83971300	-2. 84651700
C	3. 64053000	1. 99256800	1. 02267200
C	3. 74068000	3. 36896400	1. 21746000
C	4. 39360500	3. 85362800	2. 36035200
C	5. 07176100	2. 98302400	3. 20770900
C	5. 11223400	1. 62413300	2. 89008500
C	4. 39481800	1. 09419100	1. 80411100
H	-0. 22636000	4. 98053500	-3. 65527300
H	5. 69511000	0. 94346600	3. 50368400
C	3. 37697200	4. 54019000	0. 30944100
C	4. 60576900	4. 89760700	-0. 60140300
H	4. 98938500	3. 97355100	-1. 04914100
H	5. 42281700	5. 35796100	-0. 03784500
H	5. 17760300	5. 87807700	2. 26101600
H	3. 90871300	5. 67240700	3. 46221800
C	1. 04167800	3. 84028100	-0. 72385100
H	2. 00427100	6. 06251100	-3. 76633000
H	5. 58830900	3. 35245800	4. 09016600
C	4. 03216900	5. 80392200	-1. 70834800
H	4. 60259100	5. 74799700	-2. 64244400
H	4. 03080400	6. 85951700	-1. 40090300
C	4. 23142000	5. 35697700	2. 46319700
C	3. 17343800	5. 66400400	1. 37559000
H	2. 16645600	5. 57199900	1. 79806000
H	3. 26945100	6. 66827600	0. 94983500
C	4. 51715200	-0. 35837400	1. 46372300
C	4. 08804000	-1. 35347700	2. 37629100
C	5. 15028400	-0. 73617200	0. 25022100
C	3. 42647200	-1. 04252900	3. 60674600
C	4. 29936800	-2. 75004500	2. 06655100
C	5. 33830500	-2. 13704500	-0. 05200900
C	3. 03081700	-2. 02785200	4. 47295500
H	3. 21118400	-0. 00638700	3. 83382700
C	3. 86928800	-3. 74753300	2. 99667800
C	4. 91276700	-3. 10365500	0. 86291700
C	3. 26059500	-3. 39992400	4. 17178200
H	2. 51476000	-1. 76028100	5. 39040300
H	4. 03374300	-4. 79156700	2. 74067700
H	5. 06034200	-4. 15554100	0. 63122900
H	2. 93761100	-4. 16649800	4. 87133800
C	-1. 25934000	3. 41959600	-1. 78537300
C	-1. 58487400	2. 41885500	-2. 73143200

C	-2.26637300	3.95933000	-0.94811500
C	-0.60118700	1.79966000	-3.57081700
C	-2.95591500	1.98228000	-2.86855800
C	-3.62945700	3.49686400	-1.07832400
C	-0.94624100	0.86008200	-4.50766800
H	0.43992000	2.06564600	-3.43581500
C	-3.28038300	1.01159300	-3.87153400
C	-3.93967600	2.52892300	-2.03983600
C	-2.30873100	0.47452400	-4.67714200
H	-0.17551000	0.39171300	-5.11289300
H	-4.32503600	0.73360400	-3.99828200
H	-4.97325200	2.20770800	-2.15554200
H	-2.57162000	-0.24208900	-5.45195900
C	6.24255200	-0.18817200	-1.87069600
H	6.60505200	0.55756900	-2.57319600
C	5.64835800	0.21099800	-0.70198000
H	5.55631900	1.26884700	-0.48649600
C	6.39571400	-1.57000700	-2.17524300
H	6.86491800	-1.86815800	-3.10893000
C	5.96343800	-2.51336600	-1.28274600
H	6.08151300	-3.57346900	-1.49201400
C	-2.99983700	5.50215200	0.79924900
H	-2.76972800	6.27794000	1.52444200
C	-4.33965800	5.03726300	0.67203500
H	-5.11926900	5.46183800	1.29880500
C	-4.64166900	4.06370700	-0.24215400
H	-5.66224800	3.70508100	-0.35338800
C	-2.00183900	4.98422800	0.01583800
H	-0.98836400	5.35322800	0.12109300
N	0.94849700	0.96322600	1.83005100
S	-0.20338400	-0.00440400	2.25178600
O	0.11547700	-1.46037200	2.17966700
O	-1.56331400	0.31039400	1.72507500
C	-0.34318300	0.38249300	4.07239300
F	-0.81853500	1.61810600	4.23121500
F	0.83333200	0.28589900	4.69763600
F	-1.19633600	-0.48718300	4.62759400
C	-5.17624900	-1.66247600	0.68557000
C	-4.87066100	-3.09542300	1.26584300
H	-5.00520000	-3.79086500	0.43440800
H	-5.68961200	-3.32350400	1.96276100
C	-3.56547500	-3.40518700	1.98843500
C	-4.20221100	-1.31237200	-0.47191600
H	-4.39839800	-2.01766900	-1.27839300

H	-4.42368100	-0.31279100	-0.85761400
N	-2.76151600	-1.39363000	-0.18365000
C	-1.86075400	-2.03241000	-0.91292500
N	-0.64806200	-2.30213900	-0.42427300
C	0.49824600	-2.69712200	-1.19179300
C	1.14831800	-3.88285100	-0.85437600
C	0.98494200	-1.88309700	-2.21541900
C	2.28093200	-4.27102100	-1.57331700
C	2.10441200	-2.29434800	-2.93626000
H	0.52453000	-0.92133800	-2.39990500
C	2.75463700	-3.48867800	-2.62622500
H	3.63762000	-3.78731200	-3.17648400
C	2.58794000	-1.42448800	-4.06862100
C	2.95371400	-5.57530500	-1.23825100
F	2.61342300	-0.12207000	-3.72805600
F	3.82326300	-1.76957500	-4.48574600
F	1.76336700	-1.52625600	-5.14627900
F	2.89524800	-5.84467700	0.08539300
F	2.37227700	-6.61732300	-1.87557200
F	4.25975800	-5.57849300	-1.59425900
S	-2.24167500	-2.66430200	-2.54042100
H	0.78337500	-4.48753600	-0.03125600
H	-0.45766700	-2.06303600	0.56737100
H	-2.39343000	-0.86191600	0.62598300
C	-2.72423000	-4.39145800	1.60090900
H	-2.78802400	-1.51011000	-2.99326800
C	-6.59527700	-1.81521500	-0.01114500
H	-7.31164200	-2.03317100	0.78995900
H	-6.54861000	-2.72113200	-0.62100200
C	-5.27113800	-0.58407400	1.77908600
C	-4.58541100	0.63511300	1.71577200
C	-6.12387500	-0.78769200	2.88041600
C	-4.72397200	1.60208600	2.71677900
H	-3.91547800	0.86126200	0.89539700
C	-6.27309500	0.17462500	3.87548300
H	-6.68366900	-1.71443400	2.97031100
C	-5.56859100	1.37855400	3.80029100
H	-4.16128900	2.52677900	2.63523800
H	-6.93904900	-0.01852900	4.71271000
H	-5.67651600	2.12832100	4.57939100
C	-7.14435400	-0.65757600	-0.83458700
C	-7.17793400	-0.66747400	-2.18757400
C	-7.73190700	0.48425400	-0.02100000
H	-8.51386100	1.02564200	-0.55794600

H	-8.17590100	0.10289500	0.90432400
H	-6.96972300	1.20969200	0.28861300
C	-7.74311900	0.46716300	-3.01880100
H	-7.93549500	1.38101600	-2.45554600
H	-7.05151100	0.72414700	-3.83303800
H	-8.68285100	0.16487800	-3.50387000
C	-3.33376000	-2.64204000	3.27587600
H	-2.48715500	-3.02661000	3.84484600
H	-3.15090000	-1.57738100	3.10178800
H	-4.22263600	-2.69758100	3.91794600
C	-1.48590200	-4.75657700	2.41164100
H	-0.86683600	-5.47865900	1.86731000
H	-0.85891500	-3.88857200	2.63922400
H	-1.74956700	-5.22875000	3.36766400
C	-2.89783400	-5.27412200	0.38367800
H	-2.01144500	-5.21730200	-0.26420800
H	-2.97819000	-6.32737400	0.68895600
H	-3.76811300	-5.04556400	-0.23374800
C	-6.68496200	-1.79562000	-3.06974800
H	-5.80351900	-1.48324400	-3.64910600
H	-6.42089000	-2.71055100	-2.53683100
H	-7.45425700	-2.05703200	-3.80933800

INT-16-1

0 imaginary frequency

H = -5472.519877

G = -5472.736742

E(M06-2X-DCM) = -5473.494882

C	4.00022800	-2.64540400	0.53386100
C	4.55462000	-1.87830800	1.79382800
H	3.78537400	-1.16666700	2.10077000
H	4.62911500	-2.61352800	2.60622100
C	5.90182900	-1.17257700	1.70915000
C	4.00296400	-1.71205200	-0.70111500
H	3.78314700	-2.27199500	-1.61567600
H	4.99934900	-1.28555800	-0.82396500
N	3.06842300	-0.59698400	-0.58606200
C	3.21002200	0.57435300	-1.25722400
N	2.12752400	1.41513100	-1.07478200
C	1.95270700	2.76113400	-1.41955000
C	3.00682500	3.67057700	-1.61509800
C	0.63317700	3.23434500	-1.50287100
C	2.72989900	5.00354200	-1.91027200
C	0.37872700	4.57582300	-1.78670200

H	-0.19386100	2.55256300	-1.33234500
C	1.42048700	5.47535300	-2.00241600
H	1.21924300	6.51481700	-2.22858800
C	-1.04190900	5.06113100	-1.79853200
C	3.87329600	5.94773700	-2.17997900
F	-1.87506600	4.17263500	-2.39267100
F	-1.18379100	6.23768000	-2.43993000
F	-1.52521400	5.24554900	-0.53609700
F	4.20900900	5.96360800	-3.48957900
F	4.98322500	5.60967300	-1.49049700
F	3.55845200	7.22043500	-1.84163600
S	4.55507200	0.92301400	-2.21856100
H	4.02946700	3.33313200	-1.53905500
C	6.03567300	0.17215900	1.67608700
H	1.28656800	0.96356900	-0.71283900
H	2.15324000	-0.80979200	-0.19637000
H	-0.80255900	-1.96060100	1.76765100
O	-1.65808800	1.23730500	0.89820500
O	-2.80850500	-0.61050500	-0.49140500
P	-1.47858100	-0.26512500	0.34799600
O	-0.14750500	-0.37336400	-0.29660200
C	-4.70651400	2.07724200	3.63729600
C	-5.00213400	1.93393300	2.28672100
C	-3.97581600	1.77915200	1.34047100
C	-2.32864800	1.78598000	3.15283500
C	-3.37428100	2.04917600	4.05169900
C	-3.21755900	0.18778100	-1.58326000
C	-3.94329400	1.35075100	-1.33807900
C	-4.26332400	2.17631900	-2.43038100
C	-3.93667100	1.80531800	-3.72951200
C	-3.27896200	0.59592900	-3.94859500
C	-2.89379300	-0.23579300	-2.88586100
H	-3.12879800	2.19684000	5.09907600
H	-3.03512500	0.28371100	-4.95967500
C	-4.56213400	1.92129900	-0.06226900
C	-6.00369500	1.37047800	0.19369300
H	-6.71565200	1.69210000	-0.57275200
H	-5.96968000	0.27503500	0.18909900
H	-4.54591600	4.33133400	-2.46699500
H	-6.02138300	3.41174100	-2.16624800
C	-2.67569800	1.60958800	1.80061500
H	-5.50039600	2.21157900	4.36743800
H	-4.18746900	2.44996000	-4.56770500
C	-6.35617600	1.87600300	1.61174500

H	-6.83709900	2.86312100	1.57975400
H	-7.04619700	1.20564800	2.13593000
C	-4.94164800	3.44323500	-1.96444700
C	-4.64555000	3.43867000	-0.45250300
H	-5.39168900	3.97653600	0.13903800
H	-3.67409600	3.90785900	-0.27171600
C	-2.20379400	-1.53268500	-3.18313800
C	-2.95038900	-2.73532100	-3.15751200
C	-0.84351900	-1.54244200	-3.57121000
C	-4.34964200	-2.77437500	-2.85690500
C	-2.29887300	-3.98538500	-3.47629100
C	-0.20711900	-2.79886600	-3.90063000
C	-5.04509600	-3.95564700	-2.84624200
H	-4.86466300	-1.84511400	-2.63966200
C	-3.05796600	-5.19683100	-3.44184200
C	-0.94636200	-3.98301000	-3.83169500
C	-4.39193900	-5.18763700	-3.13449000
H	-6.10783500	-3.95450800	-2.61905000
H	-2.54953400	-6.12895000	-3.67717300
H	-0.46243600	-4.92533300	-4.08169100
H	-4.95866600	-6.11451200	-3.11808600
C	-0.91228400	1.72758900	3.63496100
C	0.00352200	2.73806800	3.24511100
C	-0.50537600	0.70156400	4.52432900
C	-0.35138700	3.82305200	2.38093700
C	1.35860600	2.70458400	3.74800100
C	0.85537400	0.68030000	5.01465200
C	0.55829800	4.78702100	2.03181000
H	-1.36264600	3.88495100	1.99632200
C	2.27717300	3.72920100	3.35845200
C	1.74688400	1.67774300	4.61280700
C	1.89345700	4.74222400	2.52245800
H	0.25604700	5.58930400	1.36648200
H	3.29169700	3.68350800	3.74674300
H	2.76870500	1.65774400	4.98624000
H	2.60076100	5.51354400	2.23114800
C	1.25865500	-0.39571600	-4.06112500
H	1.84265400	0.51754000	-4.11996200
C	-0.05250800	-0.35198700	-3.66575200
H	-0.50953600	0.60059000	-3.42162300
C	1.88117500	-1.63657500	-4.38170200
H	2.92355500	-1.64491900	-4.68642300
C	1.16660500	-2.80169000	-4.30148500
H	1.62650400	-3.75494800	-4.55282400

C	-0.94773800	-1.33359200	5.80753200
H	-1.63345000	-2.12169100	6.10442200
C	0.39129500	-1.34451800	6.29134400
H	0.71412700	-2.13199400	6.96697500
C	1.26383700	-0.36410700	5.90251300
H	2.28995100	-0.35845300	6.26286500
C	-1.37952200	-0.34703400	4.95914100
H	-2.40264900	-0.35893700	4.60288500
N	-1.65404200	-1.42519300	1.57436400
S	-3.01229000	-2.18650500	2.22877900
C	-3.72929200	-3.25824900	0.83616400
O	-4.03978800	-1.20325100	2.53319200
O	-2.48919300	-3.12498700	3.21368600
F	-4.21824700	-4.35923900	1.40534500
F	-4.70898300	-2.60345200	0.22506100
F	-2.77868700	-3.59259400	-0.03356400
C	2.58378600	-3.18484200	0.82433800
C	2.07920000	-3.32790000	2.12826000
C	1.75671800	-3.61497600	-0.23129700
C	0.83066100	-3.90862600	2.37171400
H	2.65615400	-2.99314600	2.98168800
C	0.51157200	-4.19690500	0.00334600
H	2.08128800	-3.49734300	-1.25868800
C	0.04741900	-4.36439200	1.30986300
H	0.47330100	-4.00583800	3.39321200
H	-0.09789500	-4.51168300	-0.83913000
H	-0.91488600	-4.82877900	1.50106900
C	4.96092400	-3.86695300	0.23245100
H	5.94448800	-3.44204700	0.00923800
H	5.07167200	-4.40570500	1.17725300
C	4.62812300	-4.84315700	-0.88543400
C	4.03355800	-6.03759900	-0.67294800
C	7.38540900	0.85550800	1.60469900
H	8.21915200	0.17519000	1.42534300
H	7.38441100	1.59498900	0.79323900
H	7.59373800	1.41169100	2.53085100
C	3.74037700	-7.01511900	-1.79006500
H	2.66595000	-7.24608600	-1.82140500
H	4.02994300	-6.65636500	-2.77914000
H	4.25326800	-7.97174600	-1.61460400
C	5.08985400	-4.43127000	-2.28015300
H	4.25360500	-4.20367800	-2.95538800
H	5.71737300	-3.53642500	-2.24153500
H	5.68367000	-5.21562800	-2.76338500

C	7.13436600	-2.06820200	1.79799300
H	7.63640000	-2.21046200	0.83142300
H	7.88218700	-1.66133600	2.48634100
H	6.87061700	-3.06289900	2.16849900
C	4.91010100	1.17821300	1.72730900
H	3.91890500	0.74859900	1.87277100
H	5.09078700	1.89089200	2.54514800
H	4.88348500	1.76799900	0.80267200
C	3.57244700	-6.55576000	0.66944900
H	3.98669700	-7.55713000	0.85388700
H	3.84227600	-5.91841600	1.51204700
H	2.47903300	-6.66151500	0.68303000

INT-16-2

0 imaginary frequency

H = -5472.520795

G = -5472.736457

E(M06-2X-DCM) = -5473.495520

C	4.03448700	-2.65282700	0.45565100
C	4.66730600	-1.85166800	1.65576000
H	3.93217200	-1.10669200	1.96773200
H	4.76045600	-2.55569100	2.49327100
C	6.02783700	-1.18935200	1.48161300
C	3.97682700	-1.76068200	-0.80922200
H	3.71668000	-2.35213200	-1.69287300
H	4.96432300	-1.33466300	-0.99249600
N	3.04115900	-0.64718600	-0.68724600
C	3.13195500	0.49839900	-1.40846400
N	2.03644300	1.32163400	-1.22404400
C	1.86072200	2.66605500	-1.57319500
C	2.91546800	3.59031000	-1.65993500
C	0.54737700	3.12142300	-1.76397000
C	2.64736800	4.92509200	-1.95170100
C	0.29992400	4.46352100	-2.05172900
H	-0.28006400	2.42504900	-1.67796200
C	1.34433300	5.37895300	-2.16018800
H	1.15042500	6.41745700	-2.39915200
C	-1.11739500	4.94507100	-2.16400200
C	3.77421200	5.92380100	-1.93976100
F	-1.93838700	4.00638400	-2.69205800
F	-1.22832900	6.05306500	-2.92383900
F	-1.63604200	5.26053900	-0.94192300
F	3.55943800	6.93498200	-2.81045400
F	4.96134100	5.36612900	-2.24340600

F	3. 90967900	6. 49472000	-0. 71206400
S	4. 42774900	0. 84603900	-2. 43476000
H	3. 93277200	3. 26306600	-1. 50435300
C	6. 19642000	0. 14781000	1. 37865100
H	1. 20241100	0. 86554600	-0. 85060900
H	2. 15057100	-0. 85110600	-0. 24048500
H	-0. 74409800	-1. 86486400	1. 87063200
O	-1. 61964000	1. 28042200	0. 84423700
O	-2. 85886300	-0. 63758100	-0. 35943500
P	-1. 48346700	-0. 25638100	0. 38600300
O	-0. 19086000	-0. 42600200	-0. 32054000
C	-4. 51282300	2. 32333700	3. 67857600
C	-4. 88047900	2. 09894600	2. 35689300
C	-3. 90646200	1. 87449600	1. 37023500
C	-2. 16550400	1. 98441200	3. 08910600
C	-3. 16023400	2. 31141500	4. 02360900
C	-3. 30833200	0. 09761000	-1. 47915800
C	-4. 01173700	1. 28165300	-1. 27326200
C	-4. 37274700	2. 04357900	-2. 39839900
C	-4. 10747000	1. 59120400	-3. 68578100
C	-3. 46945500	0. 36405600	-3. 85983200
C	-3. 04426800	-0. 40631700	-2. 76647300
H	-2. 85873400	2. 52531600	5. 04464000
H	-3. 27244800	-0. 01048800	-4. 85990400
C	-4. 56259300	1. 93678800	-0. 00697700
C	-5. 99394200	1. 42063200	0. 35529200
H	-6. 74169200	1. 70475800	-0. 39169700
H	-5. 97091400	0. 32653000	0. 41533500
H	-4. 63640100	4. 19548200	-2. 55412700
H	-6. 10511400	3. 31400900	-2. 13071800
C	-2. 58552800	1. 72168600	1. 77195900
H	-5. 26620500	2. 51020200	4. 43943500
H	-4. 38970600	2. 18700500	-4. 54970900
C	-6. 26814000	2. 01473700	1. 75664700
H	-6. 74228300	3. 00336000	1. 68930900
H	-6. 93549100	1. 38480700	2. 35506200
C	-5. 01694500	3. 34445900	-1. 98055300
C	-4. 65066900	3. 42831100	-0. 48635900
H	-5. 36310300	4. 01059200	0. 10474100
H	-3. 66762200	3. 89634200	-0. 38066500
C	-2. 37451400	-1. 72414800	-3. 01402700
C	-3. 12411700	-2. 91760300	-2. 87914800
C	-1. 03299100	-1. 76768400	-3. 46118900
C	-4. 50742000	-2. 92813600	-2. 51004500

C	-2.49394200	-4.18948500	-3.15101100
C	-0.41808800	-3.04655500	-3.74100000
C	-5.20664700	-4.10149200	-2.39415900
H	-5.00734900	-1.98374200	-2.32530600
C	-3.25594700	-5.39102300	-3.00725400
C	-1.15937100	-4.21871500	-3.56775400
C	-4.57360500	-5.35341700	-2.63800500
H	-6.25712300	-4.07886400	-2.11665900
H	-2.76343600	-6.33939900	-3.20906600
H	-0.69184200	-5.17806700	-3.78153600
H	-5.14301000	-6.27340100	-2.53828800
C	-0.72194200	1.95411200	3.48452600
C	0.16271500	2.93443500	2.96715200
C	-0.25077400	0.97994300	4.39918800
C	-0.25886700	3.97466500	2.07856000
C	1.55579900	2.91337700	3.35262300
C	1.14423100	0.97798000	4.78229200
C	0.62675800	4.89783900	1.58733800
H	-1.30191500	4.03365200	1.78967700
C	2.44845400	3.89070200	2.81014100
C	2.00658400	1.93774600	4.24633800
C	2.00405900	4.85315500	1.94437300
H	0.27306000	5.66535800	0.90656800
H	3.49524800	3.84646600	3.10075700
H	3.05612600	1.92682400	4.53326100
H	2.69359300	5.57343500	1.51429200
C	1.05407600	-0.66916200	-4.10506900
H	1.64070400	0.23440800	-4.24021900
C	-0.23985900	-0.59165200	-3.66092400
H	-0.68185400	0.37744900	-3.45787100
C	1.65484400	-1.93208900	-4.37750300
H	2.68293200	-1.96790800	-4.72593600
C	0.93703800	-3.08433300	-4.19938200
H	1.38007700	-4.05453000	-4.41333900
C	-0.59867700	-0.97133200	5.83244700
H	-1.26146500	-1.73504600	6.22861400
C	0.77365800	-0.96226100	6.21213000
H	1.14538100	-1.70947700	6.90808300
C	1.61658400	-0.01378500	5.69845400
H	2.66746200	0.00555800	5.97794200
C	-1.09174300	-0.03472500	4.96117300
H	-2.13921700	-0.06033200	4.68487600
N	-1.60127700	-1.33339600	1.69201200
S	-2.92608800	-2.03801100	2.46611500

C	-3.72055000	-3.19107100	1.18509200
O	-3.93030600	-1.02794000	2.75968000
O	-2.35548900	-2.91580400	3.48023500
F	-4.18913200	-4.24683000	1.84904100
F	-4.72406300	-2.56779200	0.57973500
F	-2.81636200	-3.59240000	0.29381500
C	2.62904900	-3.16079300	0.84261600
C	2.18604400	-3.23053600	2.17456400
C	1.74546900	-3.62860400	-0.14955600
C	0.94235600	-3.77713700	2.50617900
H	2.80710300	-2.86214700	2.98178100
C	0.50495000	-4.17717400	0.17322700
H	2.02128900	-3.56652500	-1.19585500
C	0.10211100	-4.27164100	1.50727600
H	0.63351800	-3.81681400	3.54720100
H	-0.14916000	-4.52311200	-0.62223100
H	-0.85618700	-4.71038600	1.76700100
C	4.96431100	-3.89497400	0.14469300
H	5.93829600	-3.48887500	-0.14594700
H	5.12168500	-4.40269100	1.09997800
C	4.56295500	-4.90564200	-0.91891000
C	3.96809300	-6.08449900	-0.63296400
C	7.56098100	0.78645100	1.22321700
H	7.83310200	1.35655000	2.12410000
H	8.36294300	0.07522600	1.01987500
H	7.54241200	1.50688100	0.39513300
C	3.60805200	-7.09797400	-1.69720500
H	4.11782100	-8.05442300	-1.51199300
H	2.53078100	-7.31549200	-1.66690600
H	3.85225800	-6.77940000	-2.71196500
C	4.95596800	-4.54917500	-2.34951500
H	5.59291300	-3.66054000	-2.37554000
H	5.51701900	-5.35678800	-2.83361800
H	4.08812500	-4.33679400	-2.98890600
C	7.23996600	-2.11314000	1.56624000
H	8.01971600	-1.69894500	2.21379200
H	6.96429700	-3.08553500	1.98398500
H	7.70646800	-2.30587500	0.59069100
C	5.10109300	1.18663200	1.42540900
H	5.34182700	1.94035400	2.18933700
H	5.04240100	1.72014500	0.46864300
H	4.10795200	0.79403200	1.64464100
C	3.57207400	-6.54843400	0.74944800
H	3.99358600	-7.54309900	0.95296100

H	3.88275300	-5.87910200	1.55219700
H	2.48049800	-6.65026500	0.81992200

INT-16-3

0 imaginary frequency

H = -5472.512297

G = -5472.730669

E(M06-2X-DCM) = -5473.496169

C	-4.63116400	-0.08928000	0.14919100
C	-4.68984100	1.11460600	-0.88460000
H	-4.54965900	2.02335200	-0.30061800
H	-3.80294200	1.06710500	-1.52620500
C	-5.92209800	1.29078000	-1.76829500
C	-3.90454000	0.46746300	1.40967100
H	-3.81766800	-0.29538700	2.18859600
H	-4.47279500	1.29892600	1.82778100
N	-2.57030900	0.96867000	1.11545200
C	-2.12199600	2.22210700	1.36526600
N	-0.78057100	2.35459600	1.05774500
C	0.06903500	3.46630100	1.13179800
C	-0.35628000	4.79617000	0.97268900
C	1.43775100	3.21349900	1.31456800
C	0.57307200	5.83209100	1.03328500
C	2.35282500	4.26447700	1.36505900
H	1.78604400	2.19096000	1.41846900
C	1.93142900	5.58619400	1.23815900
H	2.64005300	6.40325300	1.29846100
C	3.81850200	3.96143700	1.49013800
C	0.12373400	7.24740500	0.78139600
F	4.05300100	2.86808800	2.25298800
F	4.51226700	4.98583500	2.02525000
F	4.38419800	3.70407800	0.27519400
F	-1.17972100	7.43335300	1.05808100
F	0.30458200	7.59668800	-0.52175200
F	0.83174100	8.13526500	1.51494900
S	-3.08833800	3.45662300	2.00233900
H	-1.40280300	5.00967900	0.81430700
C	-6.86810600	2.22475100	-1.51516900
H	-0.30327100	1.47738600	0.85221300
H	-1.89040800	0.27677600	0.80774600
H	-0.23913300	-2.51214200	-1.31889300
O	1.99391300	-0.01547100	-0.87856700
O	2.19131000	-1.95081600	0.82899900
P	1.16442100	-1.16542800	-0.10998900

O	-0.03758300	-0.54149700	0.49294100
C	4.71232900	-1.23890700	-3.80050500
C	5.03420800	-1.36756000	-2.45344700
C	4.19267500	-0.83214100	-1.46385400
C	2.62956900	-0.10213500	-3.20665600
C	3.54630400	-0.56058200	-4.16599700
C	3.06981000	-1.32194700	1.72720500
C	4.26365800	-0.78866000	1.25148900
C	5.08917400	-0.10816400	2.16341600
C	4.77055700	-0.05228200	3.51608000
C	3.60255400	-0.66370200	3.97078800
C	2.71535600	-1.29726100	3.08730800
H	3.32137800	-0.39703500	-5.21575800
H	3.34834000	-0.63636700	5.02614500
C	4.92973900	-0.82748200	-0.12446300
C	5.84679700	-2.07937000	-0.31703600
H	6.71481500	-2.06483100	0.34917000
H	5.26453700	-2.98103700	-0.10250400
H	6.44248500	1.55087300	1.78970300
H	7.18705300	-0.04049600	1.62313500
C	2.96017800	-0.32309800	-1.85457700
H	5.36978500	-1.63998100	-4.56766700
H	5.41858600	0.47158100	4.21363900
C	6.22829600	-2.04758900	-1.81657400
H	7.15232200	-1.47871200	-1.98763700
H	6.39565600	-3.05030900	-2.22538900
C	6.26115200	0.52570200	1.45137200
C	5.82029900	0.46219500	-0.02418900
H	6.65606300	0.44465700	-0.72951200
H	5.20670800	1.33966100	-0.25230700
C	1.45278100	-1.92027400	3.59521300
C	1.33583800	-3.33055900	3.64457700
C	0.39736900	-1.09613100	4.05413900
C	2.38086200	-4.21328700	3.22171800
C	0.12317100	-3.92592200	4.15756000
C	-0.80970900	-1.70656600	4.56541100
C	2.23296400	-5.57429800	3.28273200
H	3.30764700	-3.79109500	2.84916000
C	0.01024300	-5.35053500	4.20492000
C	-0.91264200	-3.09943300	4.60212200
C	1.03135200	-6.15525200	3.77786100
H	3.04139100	-6.21986200	2.95079600
H	-0.91066900	-5.78039700	4.59212600
H	-1.82299600	-3.55323600	4.98929900

H	0.93255200	-7.23652400	3.81681000
C	1.40024000	0.65665700	-3.60752000
C	1.30056300	2.03255000	-3.27234500
C	0.37083900	0.03605500	-4.35829300
C	2.33509600	2.74827400	-2.58898300
C	0.12035600	2.77720800	-3.65116000
C	-0.79764300	0.79838300	-4.74064400
C	2.20262800	4.07684600	-2.27974500
H	3.24764000	2.22948800	-2.31912400
C	0.01472000	4.15777600	-3.29434800
C	-0.89648800	2.13980000	-4.36613900
C	1.02214000	4.79446500	-2.62225400
H	3.00508300	4.58344100	-1.75376400
H	-0.89134000	4.69114600	-3.57141100
H	-1.78159100	2.70649200	-4.64782700
H	0.92181100	5.83616300	-2.33416000
C	-0.59358900	1.10183700	4.46428100
H	-0.53118800	2.18504100	4.41884900
C	0.45417400	0.33543100	4.02438300
H	1.34900600	0.81763900	3.64617800
C	-1.77940500	0.49456200	4.96792400
H	-2.59992700	1.12215300	5.30268500
C	-1.87843900	-0.86979600	5.01748900
H	-2.77632300	-1.34748000	5.40351800
C	-0.58553600	-1.90484800	-5.49975500
H	-0.51190900	-2.94807200	-5.79453800
C	-1.73171700	-1.14820800	-5.87604100
H	-2.51947400	-1.61498900	-6.46093200
C	-1.83122100	0.16443200	-5.49961300
H	-2.69817300	0.75792500	-5.78070500
C	0.42176500	-1.33499200	-4.76409400
H	1.28277900	-1.92514600	-4.48317100
N	0.77655800	-2.45122400	-1.17040500
S	1.46238000	-4.02078800	-1.12723300
C	1.23190100	-4.54008700	-2.91758900
O	0.60571100	-4.91531500	-0.36064100
O	2.90003800	-3.93786400	-0.92949400
F	1.41839700	-5.85630300	-2.97027800
F	-0.00454500	-4.24936000	-3.33734300
F	2.12544600	-3.93677800	-3.69777900
C	-3.85793900	-1.32696500	-0.36026200
C	-3.43925500	-1.48825100	-1.68939700
C	-3.52339500	-2.36395000	0.53641100
C	-2.76146100	-2.63543400	-2.11711600

H	-3.63504400	-0.71912900	-2.42355400
C	-2.84384400	-3.50708200	0.12231900
H	-3.80138000	-2.28663800	1.58011000
C	-2.46916900	-3.65927000	-1.21552700
H	-2.46888600	-2.71859900	-3.16048600
H	-2.59891900	-4.27946200	0.84603100
H	-1.95845700	-4.56017000	-1.54130100
C	-6.11248100	-0.46941300	0.53873500
H	-6.59593500	0.47047700	0.83310300
H	-6.60988000	-0.77086500	-0.38385300
C	-6.38715000	-1.48902800	1.63298900
C	-6.73907100	-2.76916700	1.38093600
C	-8.08657800	2.47120400	-2.38169100
H	-8.06825600	3.49480200	-2.78239800
H	-8.19557700	1.78887400	-3.22522900
H	-9.00187100	2.39726900	-1.77783200
C	-7.05525900	-3.76414600	2.47633600
H	-8.06495700	-4.17876100	2.34446800
H	-6.36596000	-4.61950900	2.42712200
H	-6.99266200	-3.34874200	3.48351600
C	-6.33176500	-0.95314800	3.06038400
H	-5.47533500	-1.34103600	3.62915800
H	-6.24936900	0.13716800	3.06882100
H	-7.23231900	-1.20815700	3.63014600
C	-5.96209600	0.38757400	-2.98380800
H	-5.07545900	0.55069600	-3.61397500
H	-5.94362400	-0.67211500	-2.69884500
H	-6.83732400	0.53724500	-3.61662500
C	-6.86322200	3.16280200	-0.32488400
H	-6.98076400	4.20189400	-0.66273400
H	-7.72705100	2.95611000	0.32388000
H	-5.96788800	3.12134200	0.29627500
C	-6.84925600	-3.38712500	0.00576300
H	-6.65260600	-2.69412700	-0.81275400
H	-6.13817200	-4.21813400	-0.09755400
H	-7.85179600	-3.81359800	-0.14229300

INT-16-4

0 imaginary frequency

H = -5472.506757

G = -5472.726756

E(M06-2X-DCM) = -5473.478166

C	4.76715200	-0.97836400	1.93037400
C	4.57584000	-0.45337400	3.41335100

H	4. 37532100	-1. 31696200	4. 05192000
H	5. 55991000	-0. 08619200	3. 73009100
C	3. 58524000	0. 66967000	3. 72638200
C	4. 72651300	0. 17553200	0. 90436000
H	5. 03781100	-0. 19727800	-0. 07800200
H	5. 46087200	0. 93298100	1. 18798900
N	3. 42956300	0. 83288300	0. 77742300
C	3. 23224000	2. 04050200	0. 19861400
N	1. 88487400	2. 32503300	0. 05832800
C	1. 22847900	3. 50353400	-0. 31825900
C	1. 78532700	4. 79000100	-0. 24689100
C	-0. 10947000	3. 36790500	-0. 73051800
C	1. 01560200	5. 89784100	-0. 60535400
C	-0. 86190300	4. 48748500	-1. 07111100
H	-0. 56023200	2. 38262400	-0. 75765500
C	-0. 30811200	5. 76754800	-1. 02067100
H	-0. 89752600	6. 63981800	-1. 27565400
C	-2. 28262300	4. 31585500	-1. 52983700
C	1. 65082700	7. 26459500	-0. 57804100
F	-3. 07737200	5. 32732200	-1. 10470800
F	-2. 82757300	3. 16186400	-1. 07115900
F	-2. 39192200	4. 28275900	-2. 88043000
F	0. 73240000	8. 23962800	-0. 38363300
F	2. 27815300	7. 54488900	-1. 74309900
F	2. 57154600	7. 37547100	0. 40253800
S	4. 50911500	3. 02454200	-0. 30427500
H	2. 80463400	4. 92035600	0. 08551400
C	2. 30233700	0. 46777300	4. 10224100
H	1. 27178400	1. 50932300	0. 06350200
H	2. 62865000	0. 36224100	1. 18002700
H	-0. 35039900	-2. 36619200	1. 03554100
O	-2. 42778300	0. 19820300	0. 18104200
O	-1. 72329300	-1. 40230900	-1. 73612400
P	-1. 26128900	-0. 79040200	-0. 32331800
O	0. 04097900	-0. 09252500	-0. 21377900
C	-6. 29066900	-1. 27490500	0. 83684300
C	-5. 83024900	-1. 08034100	-0. 46026100
C	-4. 58887600	-0. 46690200	-0. 69602700
C	-4. 22497300	-0. 30282200	1. 71824700
C	-5. 51142200	-0. 83633100	1. 90716600
C	-1. 96248300	-0. 56623700	-2. 84735000
C	-3. 18505700	0. 08796800	-2. 94265700
C	-3. 36040100	1. 02752900	-3. 97057300
C	-2. 37383300	1. 22056300	-4. 93232300

C	-1.20725300	0.45817100	-4.87691400
C	-0.96514500	-0.44677500	-3.82993200
H	-5.88928000	-0.91865700	2.92168900
H	-0.44930300	0.56811700	-5.64652600
C	-4.48709600	-0.09914000	-2.17491300
C	-5.36620300	-1.23288800	-2.79853800
H	-5.73099900	-0.97238300	-3.79698600
H	-4.76273000	-2.14354900	-2.88229000
H	-4.60251900	2.80751300	-3.93191200
H	-5.39512500	1.38947000	-4.62049400
C	-3.76132200	-0.20453800	0.39212800
H	-7.25645100	-1.73880500	1.01983800
H	-2.51267200	1.94631300	-5.72923600
C	-6.49689100	-1.45052100	-1.76787100
H	-7.36164100	-0.80508800	-1.97395200
H	-6.86722600	-2.48172100	-1.76347300
C	-4.69720500	1.72014100	-3.83899700
C	-5.16766600	1.29204400	-2.43189800
H	-6.25605300	1.24094700	-2.33683600
H	-4.80028100	2.00843700	-1.69323700
C	0.28101500	-1.27356200	-3.82189300
C	0.19176300	-2.66725500	-4.06668700
C	1.54194700	-0.65536600	-3.64657500
C	-1.04737800	-3.33990100	-4.31596400
C	1.39931400	-3.46047400	-4.10266700
C	2.74225700	-1.46030300	-3.70293300
C	-1.09347400	-4.68871300	-4.55295300
H	-1.96633600	-2.76456100	-4.32554500
C	1.30654100	-4.86659100	-4.34530100
C	2.63689100	-2.83677000	-3.91808900
C	0.09698700	-5.46852400	-4.56147300
H	-2.04947000	-5.17091800	-4.73811300
H	2.22630900	-5.44662500	-4.35984200
H	3.54327700	-3.43796500	-3.95375200
H	0.03959700	-6.53767900	-4.74613700
C	-3.46740200	0.21236400	2.90352100
C	-3.23861200	1.60768300	3.03560800
C	-3.09406200	-0.66843100	3.94864200
C	-3.60454000	2.56169700	2.03308400
C	-2.62967200	2.11824100	4.24393000
C	-2.49488200	-0.14108300	5.15402200
C	-3.36177800	3.90124300	2.19297400
H	-4.08225500	2.21645800	1.12512000
C	-2.39947900	3.52366200	4.37545500

C	-2.28492000	1.23432500	5.27012500
C	-2.74820700	4.39363500	3.37877000
H	-3.63118500	4.59331200	1.40079800
H	-1.93662400	3.88397100	5.29103200
H	-1.83818800	1.62836000	6.18057100
H	-2.56260100	5.45851800	3.48749600
C	2.93426100	1.31667600	-3.26325700
H	3.02810100	2.38085900	-3.07213200
C	1.69570200	0.74907300	-3.40801400
H	0.80975400	1.37007500	-3.33778600
C	4.11344500	0.51991600	-3.32953600
H	5.08156800	0.99321200	-3.19785800
C	4.01579700	-0.82912800	-3.53818700
H	4.90691900	-1.45093000	-3.58480500
C	-2.90556000	-2.91489300	4.89549800
H	-3.04895000	-3.98717100	4.79841200
C	-2.33031100	-2.38793600	6.08640800
H	-2.04927300	-3.05958500	6.89291500
C	-2.13058800	-1.03924200	6.20609600
H	-1.68928000	-0.62117800	7.10782500
C	-3.27412300	-2.08593000	3.86786600
H	-3.70695600	-2.50289100	2.96794300
N	-1.26352000	-2.24415300	0.58926000
S	-1.82892400	-3.74536400	-0.01467700
C	-1.82792600	-4.73539500	1.59965000
O	-0.82294900	-4.39531500	-0.84484900
O	-3.21336000	-3.58891400	-0.43290000
F	-3.03132500	-4.69030600	2.16484800
F	-1.53501000	-5.99518800	1.28901500
F	-0.90829700	-4.26160500	2.44382800
C	3.78583200	-2.11968900	1.59108900
C	3.66627700	-3.22463700	2.45608700
C	3.04687800	-2.16360800	0.39845700
C	2.83694100	-4.30410900	2.16193200
H	4.24235500	-3.25542500	3.37668000
C	2.21261300	-3.24665200	0.09444500
H	3.11576400	-1.36031100	-0.32568700
C	2.09736300	-4.32040100	0.97671900
H	2.77532200	-5.13769100	2.85704000
H	1.66910400	-3.25535300	-0.84560500
H	1.45255100	-5.16013900	0.73458800
C	6.24686100	-1.54736900	1.88546700
H	6.89624900	-0.73164700	2.21513300
H	6.31246300	-2.31591600	2.66641200

C	6.76881300	-2.13234900	0.58097000
C	7.55610000	-1.43398800	-0.26910000
C	1.33992000	1.57603900	4.47230200
H	1.07615800	1.51137000	5.53817700
H	1.71447000	2.58235800	4.28419300
H	0.39778400	1.46547500	3.92097300
C	8.06190900	-1.99512800	-1.58210000
H	9.15132300	-2.14368200	-1.55197600
H	7.59997700	-2.94066900	-1.86991000
H	7.87541200	-1.27714900	-2.39263700
C	6.39344000	-3.58314200	0.32106400
H	7.15931500	-4.11702200	-0.24744600
H	6.26087100	-4.11906600	1.26680400
H	5.44564600	-3.68066400	-0.22274700
C	4.23993800	2.03772400	3.70690600
H	5.02026600	2.08477700	4.48073900
H	4.73634900	2.24291300	2.75218800
H	3.55172200	2.86280800	3.89124600
C	1.64917600	-0.89084000	4.22725900
H	1.16671400	-0.99118800	5.20949300
H	0.84219100	-1.00540800	3.48874000
H	2.33166800	-1.72945300	4.09513900
C	8.03277200	-0.01327100	-0.05157500
H	7.93780100	0.34026800	0.97696300
H	9.09068100	0.07299900	-0.33330400
H	7.48133100	0.69277200	-0.68804500

TS-EF-7SS

l imaginary frequency

H = -5472.489608

G = -5472.703349

E(M06-2X-DCM) = -5473.464387

O	1.13319200	-2.91234500	-0.10661500
O	3.04669000	-1.18160200	0.00960500
P	1.42166500	-1.29125500	-0.10925400
O	0.81884500	-0.59516000	1.06740100
C	2.42906000	-5.05560100	3.25250000
C	3.28571700	-4.82365400	2.18165600
C	2.83339300	-4.15814000	1.03230100
C	0.63943300	-3.88569000	2.06386800
C	1.11153900	-4.60576700	3.17407600
C	3.84936800	-1.68837500	-1.01366000
C	4.10845300	-3.05647800	-1.07347300
C	4.74726800	-3.58116100	-2.20790600

C	5.23687300	-2.73762900	-3.19942900
C	5.09406600	-1.35781000	-3.04637100
C	4.39053900	-0.80187400	-1.96548000
H	0.42673200	-4.79108200	3.99667200
H	5.51416600	-0.68481400	-3.78809500
C	3.91755300	-4.16311600	-0.03951100
C	5.19382200	-4.29338300	0.86306900
H	5.46756800	-3.29686100	1.22831000
H	6.05251500	-4.69557000	0.31678400
H	5.79759300	-5.46162100	-1.92970200
H	4.47531500	-5.55906400	-3.08701300
C	1.53452300	-3.65302200	1.00208500
H	2.77710600	-5.57527100	4.14168100
H	5.73879100	-3.14066900	-4.07561900
C	4.75093900	-5.17472600	2.04951500
H	5.31782000	-4.97024800	2.96492100
H	4.88520600	-6.24288100	1.82678300
C	4.78421500	-5.09383400	-2.14377100
C	3.81389000	-5.40699400	-0.98192900
H	2.78841100	-5.47522200	-1.36272900
H	4.04302300	-6.34441000	-0.46477600
C	4.29027100	0.68438600	-1.82702800
C	3.59389400	1.45020900	-2.79394500
C	4.96624500	1.32965000	-0.75983400
C	2.87384900	0.86016900	-3.88229700
C	3.57903800	2.89211200	-2.68570300
C	4.92481400	2.77031600	-0.65514900
C	2.22229500	1.63242400	-4.80717700
H	2.81636800	-0.21925000	-3.94736800
C	2.88404700	3.66123200	-3.67120100
C	4.23581200	3.51108600	-1.61928200
C	2.23227300	3.05265200	-4.70927700
H	1.66811000	1.15522600	-5.61028400
H	2.88613700	4.74430400	-3.57100300
H	4.20737900	4.59476100	-1.53547800
H	1.70935300	3.64735800	-5.45409600
C	-0.78458300	-3.42526600	2.05663500
C	-1.20498600	-2.42407300	2.96482000
C	-1.72651600	-4.05972100	1.21118900
C	-0.29205500	-1.71746600	3.81381300
C	-2.60432200	-2.07173500	3.04438100
C	-3.12151800	-3.69085400	1.29238400
C	-0.72723300	-0.75853600	4.69149100
H	0.76555300	-1.93668800	3.73553200

C	-3.01890700	-1.07427400	3.98365700
C	-3.52346600	-2.71390900	2.20900400
C	-2.11226400	-0.43651000	4.78670100
H	-0.00817700	-0.22856100	5.31070900
H	-4.07907000	-0.83810900	4.04707700
H	-4.57881700	-2.45643100	2.28166000
H	-2.44140600	0.31952200	5.49469600
C	6.35512200	1.27345800	1.25357400
H	6.91608400	0.70534100	1.99079700
C	5.72286800	0.62042000	0.22836500
H	5.79720700	-0.45839500	0.15688200
C	6.28855800	2.69091500	1.36458600
H	6.79382900	3.19133900	2.18641800
C	5.59829200	3.41468900	0.43042700
H	5.54220100	4.49793200	0.49575400
C	-2.30043000	-5.69593300	-0.51152600
H	-1.99595700	-6.47191000	-1.20858800
C	-3.67299600	-5.32539400	-0.43086500
H	-4.40367400	-5.82314600	-1.06306500
C	-4.06777100	-4.35232200	0.44800800
H	-5.11426200	-4.06599500	0.52446300
C	-1.36434600	-5.08799100	0.28314500
H	-0.32510500	-5.38797600	0.21551100
N	1.06392500	-0.81705500	-1.61692900
S	-0.39606300	-0.65900200	-2.17379700
O	-0.54217500	0.50991100	-3.05570400
O	-1.47419100	-0.85407400	-1.15988600
C	-0.60092800	-2.12189800	-3.31732100
F	0.35341200	-2.10921900	-4.25545500
F	-1.79665600	-2.05769900	-3.92266900
F	-0.52702500	-3.26789300	-2.63514200
C	-5.31228100	1.33369500	-0.61685900
C	-5.15698100	2.75456600	-1.27993700
H	-5.42498300	3.48527200	-0.51570300
H	-5.92507700	2.84150700	-2.06178200
C	-3.85529700	3.15768600	-1.91361000
C	-4.25273700	1.15446500	0.50455100
H	-4.45348800	1.90032900	1.27300600
H	-4.39048400	0.17227100	0.96600500
N	-2.82626800	1.28384300	0.16325500
C	-1.97113500	2.10764800	0.81283400
N	-0.69411700	1.71284500	0.94817400
C	0.37968100	2.53008900	1.41527300
C	0.73079800	3.70878500	0.75765400

C	1. 11458500	2. 09409100	2. 51825200
C	1. 78888400	4. 47734800	1. 23847200
C	2. 18194000	2. 86487000	2. 98025300
H	0. 85410700	1. 15865200	2. 99748900
C	2. 51802500	4. 06441000	2. 35446600
H	3. 34386800	4. 66077700	2. 72251900
C	3. 00731300	2. 36848900	4. 13876800
C	2. 10644500	5. 79147600	0. 57872900
F	2. 26416500	1. 64083200	5. 00622800
F	4. 02416600	1. 58053400	3. 73369000
F	3. 55265100	3. 39153500	4. 83606500
F	1. 45478700	6. 81994900	1. 16919900
F	3. 42738200	6. 08574900	0. 63878600
F	1. 75092000	5. 80275700	-0. 72712100
S	-2. 50531100	3. 66610700	1. 37230600
H	0. 19014900	4. 01871100	-0. 12673200
H	-0. 42763800	0. 71515600	0. 84623100
H	-2. 38516600	0. 47578800	-0. 30226600
C	-3. 22887400	4. 36013500	-1. 51992500
H	-2. 93493200	3. 96226600	-0. 30464100
C	-6. 71318700	1. 40716100	0. 12463400
H	-7. 47315600	1. 55967500	-0. 65201700
H	-6. 70662400	2. 32229800	0. 72280600
C	-5. 35419500	0. 20206900	-1. 65900900
C	-4. 58505700	-0. 96229400	-1. 54984800
C	-6. 23809000	0. 29285400	-2. 75162700
C	-4. 67308700	-1. 98406200	-2. 50070500
H	-3. 89051300	-1. 10364200	-0. 73271200
C	-6. 33555300	-0. 72464200	-3. 69768300
H	-6. 87030500	1. 16897800	-2. 87355900
C	-5. 54723700	-1. 87154300	-3. 57813600
H	-4. 04276300	-2. 85985100	-2. 38790800
H	-7. 02753800	-0. 61949500	-4. 52930700
H	-5. 61307100	-2. 66294400	-4. 31957500
C	-7. 14279500	0. 22781400	0. 98717000
C	-7. 08104800	0. 24981200	2. 33875300
C	-7. 72493300	-0. 94999600	0. 22237300
H	-8. 24371200	-0. 60175400	-0. 67714400
H	-6. 95214800	-1. 64680800	-0. 12429700
H	-8. 44719800	-1. 51756500	0. 81322500
C	-7. 51698200	-0. 91074500	3. 21048800
H	-6. 75852200	-1. 11302800	3. 97875300
H	-8. 44130000	-0. 66465200	3. 75329500
H	-7. 68390100	-1. 84063900	2. 66553000

C	-3.24956600	2.30614900	-2.98444300
H	-2.26721000	1.89635000	-2.71652600
H	-3.88518700	1.46553600	-3.25418800
H	-3.07512200	2.92450500	-3.87613300
C	-1.92077400	4.75484100	-2.20091300
H	-2.11087800	5.18814400	-3.19192500
H	-1.40111000	5.51587500	-1.60981600
H	-1.24167100	3.90892700	-2.33654400
C	-4.04456600	5.59339000	-1.09268300
H	-4.94835300	5.35870900	-0.52884200
H	-3.42310200	6.24393700	-0.46935100
H	-4.33593800	6.16098900	-1.98480900
C	-6.58600500	1.41037700	3.17632400
H	-5.61483000	1.17737900	3.63559700
H	-6.46992100	2.34954600	2.63235400
H	-7.28117500	1.59505200	4.00625300

TS-EF-7SS-1

1 imaginary frequency

H = -5472.489605

G = -5472.703337

E(M06-2X-DCM) = -5473.464388

O	1.13340800	-2.91239300	-0.10669200
O	3.04676400	-1.18151700	0.00961100
P	1.42174500	-1.29127700	-0.10926100
O	0.81886800	-0.59526900	1.06741600
C	2.42925700	-5.05545000	3.25255300
C	3.28595500	-4.82347300	2.18174900
C	2.83363700	-4.15804500	1.03234200
C	0.63959600	-3.88574200	2.06377300
C	1.11169800	-4.60573700	3.17403500
C	3.84950200	-1.68825300	-1.01362300
C	4.10869600	-3.05633800	-1.07339800
C	4.74760200	-3.58099500	-2.20779200
C	5.23717200	-2.73744600	-3.19931800
C	5.09425400	-1.35763400	-3.04629400
C	4.39065100	-0.80173200	-1.96543700
H	0.42686000	-4.79108100	3.99659900
H	5.51433700	-0.68462100	-3.78801300
C	3.91785200	-4.16296300	-0.03941200
C	5.19408500	-4.29308000	0.86323900
H	5.46772800	-3.29652000	1.22845100
H	6.05284000	-4.69521900	0.31701700
H	5.79810000	-5.46134000	-1.92948700

H	4. 47587800	-5. 55895300	-3. 08684600
C	1. 53472800	-3. 65303300	1. 00203700
H	2. 77729700	-5. 57505100	4. 14177700
H	5. 73915800	-3. 14046600	-4. 07547900
C	4. 75121900	-5. 17441000	2. 04970500
H	5. 31802900	-4. 96983000	2. 96513200
H	4. 88560300	-6. 24256300	1. 82703500
C	4. 78469300	-5. 09366200	-2. 14360700
C	3. 81435400	-5. 40688200	-0. 98179400
H	2. 78889800	-5. 47523000	-1. 36263200
H	4. 04356200	-6. 34425700	-0. 46459800
C	4. 29030500	0. 68452100	-1. 82697600
C	3. 59388200	1. 45032300	-2. 79387500
C	4. 96622900	1. 32979900	-0. 75976000
C	2. 87388900	0. 86026700	-3. 88225300
C	3. 57892100	2. 89222200	-2. 68558400
C	4. 92468900	2. 77045600	-0. 65502300
C	2. 22228200	1. 63250700	-4. 80710900
H	2. 81648800	-0. 21915400	-3. 94736100
C	2. 88387500	3. 66132400	-3. 67105600
C	4. 23564100	3. 51120700	-1. 61913700
C	2. 23214800	3. 05273200	-4. 70915400
H	1. 66814100	1. 15529700	-5. 61023900
H	2. 88587800	4. 74439300	-3. 57081500
H	4. 20713100	4. 59487600	-1. 53529800
H	1. 70918200	3. 64742600	-5. 45395100
C	-0. 78445700	-3. 42543900	2. 05641600
C	-1. 20502400	-2. 42426500	2. 96454500
C	-1. 72626100	-4. 05998500	1. 21089200
C	-0. 29223000	-1. 71757400	3. 81361700
C	-2. 60439500	-2. 07203600	3. 04396500
C	-3. 12129800	-3. 69122500	1. 29194600
C	-0. 72756900	-0. 75866600	4. 69123800
H	0. 76540200	-1. 93671500	3. 73544100
C	-3. 01914900	-1. 07459400	3. 98318700
C	-3. 52340900	-2. 71429400	2. 20851100
C	-2. 11263400	-0. 43674700	4. 78631000
H	-0. 00861600	-0. 22863000	5. 31052500
H	-4. 07933600	-0. 83851300	4. 04649900
H	-4. 57878500	-2. 45689500	2. 28106300
H	-2. 44190400	0. 31926600	5. 49426600
C	6. 35509000	1. 27363600	1. 25366100
H	6. 91608900	0. 70553400	1. 99086700
C	5. 72289700	0. 62058800	0. 22842100

H	5.79732100	-0.45821800	0.15689600
C	6.28840700	2.69108300	1.36473000
H	6.79362100	3.19151500	2.18659300
C	5.59809900	3.41483800	0.43059000
H	5.54191800	4.49807400	0.49595800
C	-2.29988700	-5.69627500	-0.51184600
H	-1.99528800	-6.47224300	-1.20886300
C	-3.67248800	-5.32583800	-0.43132400
H	-4.40306800	-5.82365700	-1.06358500
C	-4.06742100	-4.35277900	0.44749300
H	-5.11394000	-4.06652600	0.52383900
C	-1.36392500	-5.08824600	0.28290300
H	-0.32465500	-5.38815600	0.21537300
N	1.06397000	-0.81705800	-1.61692300
S	-0.39604200	-0.65892200	-2.17370300
O	-0.54222000	0.51016000	-3.05537900
O	-1.47414000	-0.85421800	-1.15980300
C	-0.60091000	-2.12160000	-3.31749800
F	0.35328400	-2.10862600	-4.25577500
F	-1.79674000	-2.05740000	-3.92265000
F	-0.52678300	-3.26772600	-2.63556700
C	-5.31240000	1.33352700	-0.61664700
C	-5.15716200	2.75437800	-1.27979400
H	-5.42501300	3.48511400	-0.51553800
H	-5.92538300	2.84130900	-2.06151800
C	-3.85557000	3.15742600	-1.91369500
C	-4.25273300	1.15429200	0.50464800
H	-4.45344100	1.90012300	1.27314500
H	-4.39041800	0.17208100	0.96608400
N	-2.82629600	1.28372100	0.16324700
C	-1.97116100	2.10757900	0.81277000
N	-0.69413800	1.71278000	0.94811400
C	0.37964100	2.53005700	1.41519600
C	0.73072700	3.70874700	0.75755000
C	1.11453200	2.09412500	2.51820800
C	1.78874300	4.47738800	1.23839500
C	2.18183000	2.86497400	2.98022700
H	0.85408100	1.15868900	2.99746400
C	2.51786300	4.06452400	2.35443100
H	3.34364200	4.66095900	2.72251900
C	3.00718100	2.36867000	4.13879200
C	2.10624900	5.79152400	0.57863600
F	2.26404300	1.64096200	5.00621700
F	4.02412200	1.58079100	3.73378200

F	3.55239700	3.39176700	4.83611000
F	1.45462400	6.81998900	1.16915500
F	3.42719000	6.08581300	0.63861100
F	1.75064600	5.80281000	-0.72719300
S	-2.50534800	3.66606700	1.37210500
H	0.19010400	4.01861100	-0.12687300
H	-0.42766900	0.71508700	0.84623800
H	-2.38518300	0.47564800	-0.30222800
C	-3.22902700	4.35986200	-1.52011600
H	-2.93507000	3.96209000	-0.30503300
C	-6.71321400	1.40706000	0.12501100
H	-7.47327100	1.55956000	-0.65155500
H	-6.70655900	2.32222700	0.72313400
C	-5.35446200	0.20189100	-1.65878000
C	-4.58519500	-0.96240600	-1.54981200
C	-6.23860900	0.29262100	-2.75120000
C	-4.67334000	-1.98416000	-2.50067700
H	-3.89045100	-1.10370900	-0.73284000
C	-6.33619100	-0.72486400	-3.69725500
H	-6.87092800	1.16869300	-2.87297300
C	-5.54774200	-1.87169500	-3.57791000
H	-4.04290600	-2.85989100	-2.38804300
H	-7.02837200	-0.61976400	-4.52872100
H	-5.61367000	-2.66308500	-4.31935300
C	-7.14277300	0.22776900	0.98766100
C	-7.08077800	0.24981500	2.33923600
C	-7.51663900	-0.91063200	3.21115400
H	-8.44072400	-0.66434000	3.75426600
H	-7.68391200	-1.84052100	2.66630000
H	-6.75795700	-1.11303000	3.97917100
C	-1.92100000	4.75444200	-2.20132800
H	-1.40126800	5.51557700	-1.61042300
H	-1.24191900	3.90849700	-2.33687800
H	-2.11121300	5.18756100	-3.19239800
C	-3.24999700	2.30581400	-2.98454800
H	-3.88566300	1.46519100	-3.25414500
H	-3.07569300	2.92413000	-3.87629500
H	-2.26760100	1.89603400	-2.71675200
C	-7.72516200	-0.94995500	0.22294300
H	-8.24476800	-0.60153500	-0.67603700
H	-6.95243900	-1.64639100	-0.12460500
H	-8.44678500	-1.51796500	0.81414400
C	-4.04461000	5.59321800	-1.09293700
H	-4.94833700	5.35865000	-0.52895500

H	-3.42303300	6.24380100	-0.46975900
H	-4.33606200	6.16071000	-1.98510400
C	-6.58544700	1.41037700	3.17664800
H	-5.61424000	1.17727000	3.63579700
H	-6.46929900	2.34948900	2.63259500
H	-7.28047000	1.59521000	4.00666400

TS-EF-7SS-2

l imaginary frequency

H = -5472.478282

G = -5472.691983

E(M06-2X-DCM) = -5473.459087

O	2.53791300	-1.38140600	-0.39501600
O	1.74115400	0.72384000	-1.69522600
P	1.26150100	-0.37950200	-0.56767100
O	0.90931600	0.41125700	0.65553700
C	6.43389700	-0.05341900	0.38141400
C	5.90796300	0.00809600	-0.90405300
C	4.62744200	-0.49600600	-1.18320100
C	4.35379600	-1.07209100	1.17686600
C	5.66823400	-0.62197000	1.39638000
C	1.90041900	0.30690800	-3.01763200
C	3.05614600	-0.37447100	-3.38975400
C	3.11840600	-0.97619100	-4.65706000
C	2.10092300	-0.78304600	-5.58413200
C	1.01927700	0.02918500	-5.24160800
C	0.88627300	0.57925300	-3.95692000
H	6.08207600	-0.71524100	2.39575900
H	0.24092700	0.23061600	-5.97178000
C	4.40589400	-0.51697500	-2.69452700
C	5.35730000	0.65178300	-3.12698700
H	4.83071200	1.60311900	-2.98521700
H	5.64671600	0.58642100	-4.18003300
H	5.10465900	-1.32746400	-5.46364200
H	4.17838300	-2.80080400	-5.19842600
C	3.83563500	-0.95839600	-0.13001700
H	7.43302100	0.31957500	0.59281400
H	2.14764200	-1.24438900	-6.56730800
C	6.54967000	0.56740000	-2.15389000
H	7.02897400	1.53838300	-1.98273500
H	7.33071800	-0.10554600	-2.53487700
C	4.37907300	-1.80394200	-4.78958200
C	4.90266700	-1.85557000	-3.33623300
H	4.43345400	-2.69165500	-2.80802400

H	5.98833500	-1.97659600	-3.26812200
C	-0.26235700	1.49403000	-3.66883900
C	-1.59321800	1.00901300	-3.67532900
C	-0.01134600	2.88068900	-3.50507000
C	-1.90929800	-0.38213800	-3.80576700
C	-2.69322700	1.93786100	-3.52837200
C	-1.11977400	3.79324700	-3.33711600
C	-3.20853200	-0.81760400	-3.82103200
H	-1.10262400	-1.10153500	-3.85419100
C	-4.03500000	1.44271700	-3.56468100
C	-2.42725900	3.29861800	-3.35663300
C	-4.28898100	0.10554000	-3.71615600
H	-3.41784000	-1.88079700	-3.87972400
H	-4.85002700	2.15683700	-3.46950000
H	-3.25903900	3.99267100	-3.24994900
H	-5.31049500	-0.26315700	-3.73278800
C	3.61312100	-1.68719300	2.32189200
C	3.40185900	-0.93091100	3.50373300
C	3.24254000	-3.05607200	2.28044400
C	3.72768200	0.46147800	3.61041400
C	2.83807500	-1.57051100	4.67182000
C	2.62679900	-3.66443000	3.43873600
C	3.58274600	1.14480300	4.79046300
H	4.08515700	0.98504700	2.73167700
C	2.70130400	-0.82190200	5.88372700
C	2.45141400	-2.91098100	4.60197000
C	3.07837200	0.49338000	5.95234900
H	3.83968800	2.19964700	4.83422300
H	2.29981700	-1.33081200	6.75750900
H	2.01834700	-3.38573900	5.48046400
H	2.98582700	1.04456300	6.88491000
C	1.51588400	4.79068700	-3.38809800
H	2.52727700	5.18698300	-3.42222800
C	1.30625200	3.44398600	-3.53561100
H	2.15215600	2.78553600	-3.69504400
C	0.41995000	5.68157800	-3.20721900
H	0.60281900	6.74795400	-3.10408100
C	-0.85838800	5.19152300	-3.18679500
H	-1.70628200	5.86154000	-3.07000800
C	3.10094800	-5.21152100	1.13849200
H	3.28078800	-5.81707800	0.25472100
C	2.46228300	-5.79386800	2.26860200
H	2.15797600	-6.83634900	2.23799300
C	2.23976200	-5.03993000	3.38761100

H	1.76499000	-5.47297800	4.26489100
C	3.48151100	-3.89622500	1.14690300
H	3.96903300	-3.47948800	0.27500000
N	0.08524200	-1.25879100	-1.23983900
S	-0.22538500	-2.82749500	-1.14141500
O	-1.55931900	-3.06780700	-1.70587400
O	0.11876000	-3.43814000	0.15098100
C	0.90035300	-3.66282700	-2.39011900
F	0.81410000	-3.05296300	-3.58163700
F	0.51547100	-4.93537700	-2.53245600
F	2.18560300	-3.65315600	-2.00218200
C	-0.81213900	3.93314700	2.40577400
C	-1.12060900	3.32670700	3.83086100
H	-2.06541700	3.75619500	4.16101200
H	-0.36139900	3.70385700	4.52926400
C	-1.15596200	1.83731500	4.02008400
C	-1.68787600	3.22995800	1.33927100
H	-2.73659900	3.40499600	1.57939400
H	-1.50266800	3.69053700	0.36358200
N	-1.52186100	1.77593300	1.20391600
C	-2.54024100	0.89231600	1.13234800
N	-2.32646300	-0.26531900	0.48698000
C	-3.24292400	-1.37042400	0.45971300
C	-2.96517900	-2.51049900	1.21095300
C	-4.35441300	-1.32315300	-0.37672800
C	-3.82308600	-3.60743100	1.13128300
C	-5.20020200	-2.42923900	-0.45518500
H	-4.54388600	-0.43772300	-0.97164600
C	-4.94247500	-3.57231800	0.30050100
H	-5.60798500	-4.42552500	0.24506600
C	-6.35557200	-2.39815400	-1.41923100
C	-3.50930400	-4.86200200	1.90484600
F	-5.95644200	-2.67621200	-2.68555000
F	-7.30966300	-3.29750200	-1.10059200
F	-6.94048300	-1.17892900	-1.46129300
F	-2.81506100	-4.59126500	3.03293000
F	-4.64148800	-5.50853700	2.27348800
F	-2.77775900	-5.73107700	1.18245100
S	-4.03438600	1.17579200	1.97729900
H	-2.07515600	-2.55374000	1.82756200
H	-1.46670600	-0.39780700	-0.06379600
H	-0.60227100	1.42063300	0.88603900
C	-2.31856300	1.20637800	4.51501200
H	-2.99307000	1.25284900	3.38905500

C	-1.33089900	5.42836600	2.50460200
H	-0.70543100	5.92724500	3.25652100
H	-2.33634000	5.38555800	2.93056900
C	0.69331000	3.94208200	2.07598600
C	1.61511700	4.44272100	3.01532200
C	1.19916600	3.54642700	0.83137800
C	2.97473700	4.53591200	2.72681800
H	1.27406800	4.78518000	3.98917300
C	2.56324100	3.62801900	0.53900900
H	0.54908000	3.15994400	0.05664000
C	3.45856000	4.12369300	1.48239600
H	3.65541900	4.93544500	3.47442800
H	2.90888500	3.28991100	-0.43268900
H	4.51922800	4.18924600	1.25594600
C	-1.34864500	6.28749400	1.25096300
C	-2.48908500	6.59348900	0.59230900
C	-0.01012000	6.87439400	0.82224200
H	0.74501400	6.74484400	1.60096900
H	0.38284000	6.39301300	-0.08181400
H	-0.08632200	7.94756900	0.61551600
C	0.08902600	1.05682100	3.74560400
H	-0.09739400	0.11688400	3.22174200
H	0.82472800	1.61453200	3.17112300
H	0.54489600	0.78542400	4.71076300
C	-2.25345800	-0.27692000	4.87941400
H	-1.74120300	-0.41790500	5.83987500
H	-3.26435900	-0.68267100	4.97901300
H	-1.72844800	-0.87719900	4.13338200
C	-2.50381000	7.51222100	-0.61162400
H	-3.17500000	7.11902900	-1.38620900
H	-2.89734100	8.50297800	-0.33919100
H	-1.52146000	7.65406000	-1.06424600
C	-3.87844300	6.11247100	0.94909600
H	-4.26231400	5.43062600	0.17713600
H	-3.95191000	5.59269300	1.90616800
H	-4.57483200	6.96169200	0.98106300
C	-3.34198600	1.95808900	5.38337600
H	-3.58061600	2.96102300	5.02601700
H	-4.27768600	1.39129200	5.40554400
H	-2.97515100	2.03751200	6.41396500

TS-EF-7SS-3

l imaginary frequency

H = -5472.487369

G = -5472.700788

E(M06-2X-DCM) = -5473.463181

O	0.89330600	-2.96334200	-0.15961700
O	2.91796700	-1.35776900	-0.15090100
P	1.28412800	-1.36421500	-0.18341600
O	0.79265000	-0.63162700	1.02287800
C	2.30325000	-5.26260100	3.04716800
C	3.08486800	-5.06535500	1.91384500
C	2.59119300	-4.34108600	0.81823700
C	0.51208000	-3.94233500	2.03097800
C	1.02012600	-4.71873500	3.08605800
C	3.62657600	-1.88432000	-1.23183300
C	3.78105200	-3.26411400	-1.34973000
C	4.30408500	-3.79301700	-2.53994300
C	4.79156800	-2.95183600	-3.53464700
C	4.76739900	-1.57169500	-3.32690700
C	4.17769200	-1.00566500	-2.18501300
H	0.39277800	-4.87419400	3.95911400
H	5.19280300	-0.90498000	-4.07132900
C	3.58617200	-4.38871600	-0.33624700
C	4.91614000	-4.63450800	0.45925800
H	5.28826200	-3.67059600	0.82508000
H	5.69864700	-5.07909600	-0.16318800
H	5.22685200	-5.75427800	-2.39729000
H	3.82118400	-5.71326100	-3.45530200
C	1.33226500	-3.74774800	0.90301200
H	2.68376700	-5.82700000	3.89479600
H	5.20370000	-3.35805300	-4.45508400
C	4.50509300	-5.51637800	1.65608400
H	5.15592400	-5.38020600	2.52729200
H	4.54199600	-6.58438300	1.39791100
C	4.23139200	-5.30595500	-2.52395300
C	3.32574100	-5.58977100	-1.30308800
H	2.27344500	-5.57374000	-1.60901300
H	3.52371400	-6.55777100	-0.83130200
C	4.21022200	0.47672000	-1.98369800
C	3.51764300	1.33941100	-2.86822600
C	5.00869200	1.01675900	-0.94271800
C	2.67961100	0.85884300	-3.92522100
C	3.63190600	2.77165200	-2.70317800
C	5.09864200	2.44999800	-0.78136500
C	2.03331900	1.72204700	-4.77004800
H	2.52963200	-0.20855500	-4.02883500
C	2.93691300	3.63810500	-3.60424800

C	4. 41163300	3. 28681500	-1. 66484100
C	2. 16719800	3. 13098100	-4. 61607100
H	1. 38738800	1. 32753500	-5. 54885300
H	3. 03584900	4. 71180700	-3. 46130600
H	4. 48335000	4. 36433400	-1. 53924400
H	1. 64621700	3. 79890000	-5. 29762300
C	-0. 87260000	-3. 38682700	2. 15295200
C	-1. 14221200	-2. 37373000	3. 10409200
C	-1. 92689100	-3. 94778100	1. 39286800
C	-0. 11123800	-1. 74060200	3. 87171200
C	-2. 50250400	-1. 93381900	3. 31603700
C	-3. 28182900	-3. 49205000	1. 60583900
C	-0. 40060000	-0. 76862000	4. 79405600
H	0. 91811300	-2. 02722600	3. 69507000
C	-2. 76333400	-0. 92543200	4. 29782000
C	-3. 53371600	-2. 50484000	2. 56400600
C	-1. 74696200	-0. 35891600	5. 01848600
H	0. 40525400	-0. 29454300	5. 34792700
H	-3. 79482100	-0. 62026100	4. 46122100
H	-4. 56007000	-2. 18563000	2. 73806600
H	-1. 95982500	0. 40733400	5. 75918100
C	6. 51959200	0. 75851400	0. 96444100
H	7. 07777400	0. 11430300	1. 63851100
C	5. 76585700	0. 20516400	-0. 03709200
H	5. 74202300	-0. 87201500	-0. 15353800
C	6. 58343100	2. 17048000	1. 13239900
H	7. 18421300	2. 59124200	1. 93437100
C	5. 89670400	2. 98876300	0. 27694400
H	5. 93826200	4. 06918100	0. 38627300
C	-2. 76101800	-5. 52257300	-0. 28006700
H	-2. 57266700	-6. 30710200	-1. 00788500
C	-4. 09380800	-5. 06737400	-0. 06908500
H	-4. 91024500	-5. 51099000	-0. 63306500
C	-4. 34250400	-4. 08156700	0. 84850500
H	-5. 35677000	-3. 72982700	1. 02376100
C	-1. 71850000	-4. 98455100	0. 42771300
H	-0. 71098400	-5. 34745400	0. 26075000
N	0. 87742000	-0. 87227900	-1. 67223600
S	-0. 59443000	-0. 60674500	-2. 15592100
O	-0. 67835100	0. 51804200	-3. 09943100
O	-1. 61964800	-0. 63865600	-1. 07223900
C	-1. 01437600	-2. 10195600	-3. 19590000
F	-0. 10420000	-2. 25623300	-4. 16457400
F	-2. 21826300	-1. 93366300	-3. 76258100

F	-1.04437900	-3.20755800	-2.44613700
C	-5.15718300	1.80158700	-0.35025200
C	-4.92204500	3.21341500	-1.00560500
H	-5.14814200	3.95010900	-0.23422800
H	-5.68346100	3.36013400	-1.78476200
C	-3.59923700	3.55138700	-1.63487000
C	-4.08592100	1.57190200	0.74766100
H	-4.20497000	2.34581300	1.50595900
H	-4.26976700	0.60970200	1.23252000
N	-2.67082200	1.59149300	0.34590600
C	-1.72034700	2.32030300	0.97838900
N	-0.47613200	1.81617800	1.03564100
C	0.68337900	2.52046000	1.48075500
C	1.09847600	3.69897900	0.86033500
C	1.43435700	1.97149900	2.52079900
C	2.24075700	4.35302200	1.31675400
C	2.58490300	2.62893100	2.95861800
H	1.12116400	1.03704400	2.96974000
C	2.98868000	3.82650900	2.37097700
H	3.87994500	4.33353600	2.71947000
C	3.42179800	2.00734900	4.04640000
C	2.63653400	5.66642600	0.69923400
F	2.65645400	1.34751000	4.94923700
F	4.30690500	1.11623300	3.55588200
F	4.12993000	2.93839800	4.72533700
F	2.10427000	6.71637900	1.36611800
F	3.97925400	5.84656900	0.70292900
F	2.22110100	5.76902200	-0.58511300
S	-2.09689200	3.89652000	1.60976400
H	0.54127600	4.09768400	0.02311800
H	-0.30248700	0.80249700	0.89077000
H	-2.32723000	0.75867200	-0.15902300
C	-2.90909000	4.71728900	-1.23052600
H	-2.58940100	4.27658600	-0.04724500
C	-6.55694900	1.94146100	0.39368000
H	-7.30941700	2.07387500	-0.38885800
H	-6.53017500	2.88613400	0.95347000
C	-5.27689100	0.66277200	-1.37849500
C	-4.73009700	-0.60777600	-1.16150400
C	-6.03148700	0.84664700	-2.55315600
C	-4.90562100	-1.64318700	-2.08424600
H	-4.13744200	-0.82103600	-0.28103100
C	-6.21243800	-0.18122800	-3.47516400
H	-6.49647000	1.80650300	-2.76279000

C	-5.64595000	-1.43669100	-3.24496600
H	-4.44349000	-2.60499500	-1.88657200
H	-6.79603000	0.00090900	-4.37386400
H	-5.77427200	-2.23850400	-3.96676500
C	-6.97758200	0.84418300	1.36098400
C	-7.78869400	-0.18231900	1.02406100
C	-8.18956300	-1.25626200	2.01298100
H	-8.06370900	-2.25015000	1.56259400
H	-7.61752200	-1.23945500	2.94229900
H	-9.25529400	-1.17068700	2.27117000
C	-1.60602300	5.07663600	-1.94205300
H	-1.04132800	5.80419200	-1.35047800
H	-0.96183000	4.21117500	-2.11654300
H	-1.80938200	5.53766500	-2.91766600
C	-3.04203900	2.68409600	-2.71896300
H	-3.67009300	1.82351500	-2.93487800
H	-2.93895800	3.28839300	-3.63270400
H	-2.03711500	2.30298900	-2.50604900
C	-6.49192300	1.01506500	2.79801900
H	-5.70422000	0.30176700	3.07544000
H	-6.08098600	2.01607200	2.96087800
H	-7.30589300	0.88646100	3.51926200
C	-3.65837600	5.97506400	-0.75491200
H	-4.53577800	5.76900000	-0.14056900
H	-2.98028900	6.59786900	-0.16334800
H	-3.97899000	6.56036000	-1.62526300
C	-8.40933000	-0.40083100	-0.33537900
H	-9.46638900	-0.67720800	-0.22175100
H	-8.35751300	0.46811900	-0.99225600
H	-7.91954100	-1.23107500	-0.86105600

TS-EF-7SS-4

l imaginary frequency

H = -5472.488744

G = -5472.702262

E(M06-2X-DCM) = -5473.462508

O	1.82991500	-2.68180900	0.02983900
O	3.25132600	-0.52464200	0.04279900
P	1.70567200	-1.04257900	-0.06585700
O	0.93418200	-0.45464000	1.07080800
C	3.63375500	-4.26992100	3.46248900
C	4.40035800	-3.88690300	2.36710100
C	3.79146100	-3.40867800	1.19707000
C	1.60407300	-3.63506500	2.25317500

C	2. 24587100	-4. 16131100	3. 38699800
C	4. 15959400	-0. 85777500	-0. 96340700
C	4. 74665600	-2. 12162700	-0. 97186500
C	5. 49367800	-2. 52004300	-2. 09135700
C	5. 76226800	-1. 62282300	-3. 11962000
C	5. 28873400	-0. 31390600	-3. 01741400
C	4. 47061400	0. 09629000	-1. 95214100
H	1. 63258200	-4. 46864700	4. 22922100
H	5. 53327000	0. 41157000	-3. 78777600
C	4. 83754000	-3. 19587000	0. 10855700
C	6. 11196800	-2. 96796200	0. 99468100
H	6. 13465500	-1. 91904000	1. 31194400
H	7. 03994900	-3. 17194500	0. 45179900
H	6. 97225900	-4. 07496800	-1. 75428700
H	5. 70866200	-4. 53950400	-2. 88770100
C	2. 40766500	-3. 24132400	1. 16606400
H	4. 10433800	-4. 64472800	4. 36796900
H	6. 34666200	-1. 92591900	-3. 98488800
C	5. 90598400	-3. 87499300	2. 22534500
H	6. 41116900	-3. 49632700	3. 12119200
H	6. 29619000	-4. 88713400	2. 04660100
C	5. 89886200	-3. 97424100	-1. 96798700
C	5. 03915200	-4. 46621400	-0. 78084700
H	4. 06057500	-4. 80043300	-1. 14405700
H	5. 49386000	-5. 29558400	-0. 22937200
C	4. 01579500	1. 51910900	-1. 86711100
C	3. 15666300	2. 05926600	-2. 85536900
C	4. 51797400	2. 34745400	-0. 83061600
C	2. 59740200	1. 27297700	-3. 91364100
C	2. 79907100	3. 45944300	-2. 80135600
C	4. 13560700	3. 74014800	-0. 78057400
C	1. 77971800	1. 83146300	-4. 86017500
H	2. 79893000	0. 20925700	-3. 93746700
C	1. 93957700	4. 00213100	-3. 80756300
C	3. 29090500	4. 25805100	-1. 76600900
C	1. 45069500	3. 21580600	-4. 81538700
H	1. 35406700	1. 20512500	-5. 63873500
H	1. 68314500	5. 05744700	-3. 74762900
H	3. 00711800	5. 30672600	-1. 72396400
H	0. 80034800	3. 63950400	-5. 57661800
C	0. 11000900	-3. 54473900	2. 25441600
C	-0. 53800600	-2. 63827200	3. 12745800
C	-0. 65178900	-4. 43892300	1. 46410700
C	0. 17773300	-1. 67865000	3. 91500200

C	-1.97911800	-2.65335000	3.23491300
C	-2.09337400	-4.43426300	1.56877000
C	-0.47332000	-0.82114200	4.76355500
H	1.25431500	-1.62211400	3.81230400
C	-2.61900800	-1.75295900	4.14526900
C	-2.71637800	-3.54991400	2.45541500
C	-1.89213300	-0.86431000	4.89069500
H	0.09608600	-0.09228900	5.33426900
H	-3.70223600	-1.79626800	4.23463800
H	-3.80072700	-3.57289500	2.55267100
H	-2.39142000	-0.18563800	5.57725800
C	5.87826500	2.70146800	1.17210200
H	6.55731800	2.31191200	1.92581200
C	5.42031400	1.87743600	0.17783700
H	5.74889800	0.84519100	0.14714200
C	5.47717300	4.06594400	1.22928300
H	5.84844000	4.70383700	2.02702800
C	4.63578500	4.56804700	0.27380400
H	4.32410700	5.60884100	0.29791000
C	-0.81557800	-6.25151100	-0.16737300
H	-0.33402400	-6.95805300	-0.83789900
C	-2.23580700	-6.23904600	-0.06451100
H	-2.82497600	-6.93732900	-0.65323900
C	-2.85245900	-5.35572400	0.78097200
H	-3.93609300	-5.34092300	0.87254000
C	-0.05352900	-5.38614000	0.57273300
H	1.02660500	-5.41398400	0.48860100
N	1.26124600	-0.75918500	-1.59804200
S	-0.18676600	-0.99227100	-2.16114100
O	-0.58622500	0.03779000	-3.13249300
O	-1.20367500	-1.35403800	-1.13033400
C	-0.03147700	-2.54792100	-3.18417200
F	0.91603000	-2.39166400	-4.11622700
F	-1.19699600	-2.80332400	-3.79679900
F	0.28446600	-3.59128900	-2.41176700
C	-5.43013800	-0.16389900	-0.72119600
C	-5.62903200	1.21223500	-1.44602400
H	-6.07685900	1.88302800	-0.71565200
H	-6.37982000	1.07723800	-2.23807100
C	-4.45505800	1.90251300	-2.08590500
C	-4.39153100	0.00254900	0.41930500
H	-4.79816000	0.71885800	1.13262100
H	-4.28042100	-0.95251300	0.94340300
N	-3.03710800	0.46228700	0.07288500

C	-2.41273300	1.49540100	0.68571700
N	-1.08015800	1.42426200	0.84177400
C	-0.23851700	2.49245200	1.27738500
C	-0.17455100	3.69704200	0.57705300
C	0.56997600	2.28506100	2.39552300
C	0.66564100	4.71270000	1.02860500
C	1.41890200	3.30460300	2.82788800
H	0.53674400	1.33218700	2.90898000
C	1.46413500	4.52611600	2.15791500
H	2.12169100	5.31480200	2.50221800
C	2.32908300	3.06020400	4.00333600
C	0.66502000	6.04038500	0.32130900
F	1.76012800	2.23114700	4.91131000
F	3.49506300	2.49462700	3.63060900
F	2.63373800	4.21095900	4.64581200
F	-0.22390600	6.90076900	0.86961400
F	1.87475900	6.64757100	0.37638100
F	0.33503500	5.91912500	-0.98563100
S	-3.31314800	2.90312500	1.16711800
H	-0.76733800	3.83796500	-0.31698900
H	-0.58211100	0.51555400	0.78432600
H	-2.41014200	-0.23543200	-0.35746200
C	-4.16737000	3.24347800	-1.75190300
H	-3.79757400	2.99481700	-0.51449300
C	-6.80002300	-0.55547400	-0.01120900
H	-6.61684300	-1.52303200	0.46528800
H	-7.51667200	-0.76185200	-0.81382600
C	-5.14742900	-1.33147100	-1.68728500
C	-4.16265300	-2.29639100	-1.44424700
C	-5.96440700	-1.51344500	-2.82008300
C	-3.97493300	-3.37757900	-2.31078400
H	-3.50193400	-2.22445400	-0.59014100
C	-5.78683100	-2.59249300	-3.68238800
H	-6.75791200	-0.80421700	-3.04232800
C	-4.78353100	-3.53146200	-3.43294000
H	-3.18314300	-4.08806600	-2.09735000
H	-6.43288500	-2.69756600	-4.55016600
H	-4.63470500	-4.36895100	-4.10886200
C	-7.44918100	0.41387700	0.96647200
C	-7.31251600	0.32855400	2.30839100
C	-7.99755000	1.28607200	3.25885400
H	-7.27777400	1.67739800	3.99003900
H	-8.46382000	2.13965000	2.76420600
H	-8.77456000	0.76676800	3.83843200

C	-2.99277400	3.93092200	-2.44372400
H	-2.70260800	4.83048600	-1.89126600
H	-2.11346600	3.28679800	-2.52748600
H	-3.26762400	4.24770500	-3.45864200
C	-3.62636800	1.18532700	-3.10480900
H	-4.00363600	0.18812000	-3.31997400
H	-3.61740100	1.77313900	-4.03376800
H	-2.57314700	1.07593800	-2.81809100
C	-8.37824700	1.45510900	0.34682300
H	-8.47812800	1.30541400	-0.73211600
H	-9.38829600	1.39654000	0.76926000
H	-8.03247300	2.48593700	0.50060900
C	-5.27980600	4.24385700	-1.39221900
H	-6.11153500	3.80796100	-0.83737000
H	-4.86203800	5.05385800	-0.78591500
H	-5.67877100	4.68589000	-2.31340900
C	-6.49784600	-0.71506500	3.03829100
H	-7.08502400	-1.13850000	3.86411800
H	-6.16800800	-1.54371800	2.40872600
H	-5.60310300	-0.26669900	3.49237700

TS-EF-7SS-5

l imaginary frequency

H = -5472.489149

G = -5472.703157

E(M06-2X-DCM) = -5473.463843

O	1.98612900	-2.61320000	0.04165400
O	3.31951900	-0.39918100	0.00242100
P	1.79442600	-0.98047900	-0.06667400
O	1.02867400	-0.41439200	1.08498600
C	3.89601400	-4.06170700	3.47952100
C	4.63306900	-3.66231200	2.36986100
C	3.99108500	-3.23420100	1.19799600
C	1.82704200	-3.54848400	2.27926000
C	2.50377600	-4.02319400	3.41534500
C	4.22283100	-0.71252400	-1.01397400
C	4.86491500	-1.94913000	-1.00624400
C	5.61437400	-2.33697200	-2.12760900
C	5.82789700	-1.45015600	-3.17767700
C	5.29617600	-0.16230000	-3.09564400
C	4.47541600	0.23341700	-2.02680800
H	1.91375400	-4.34721900	4.26791400
H	5.49656600	0.55680100	-3.88450800
C	5.01598800	-2.99520200	0.09456500

C	6.28691700	-2.69131400	0.96225700
H	6.26413200	-1.63632300	1.25866900
H	7.21793800	-2.86323300	0.41346700
H	7.16733300	-3.81424900	-1.77727500
H	5.91342200	-4.36119000	-2.88439700
C	2.60057400	-3.13199900	1.17854700
H	4.39243400	-4.39695300	4.38671400
H	6.41410500	-1.74437400	-4.04478500
C	6.13513700	-3.58218500	2.21253400
H	6.62990800	-3.16216700	3.09567300
H	6.57117800	-4.57820900	2.04992900
C	6.08794700	-3.76794500	-1.97931000
C	5.26619800	-4.27345100	-0.77115900
H	4.30002400	-4.66020300	-1.11491300
H	5.76532000	-5.06907900	-0.20849800
C	3.95623400	1.63519700	-1.96428000
C	3.06066800	2.11435000	-2.95161900
C	4.43165500	2.50710800	-0.95124500
C	2.52802200	1.28189500	-3.98808900
C	2.63665900	3.49654300	-2.91942100
C	3.98232500	3.88027600	-0.92171800
C	1.67536800	1.78256400	-4.93604200
H	2.77922500	0.22851800	-3.99356700
C	1.74285400	3.97826600	-3.92673700
C	3.10010300	4.33732300	-1.90444700
C	1.28204600	3.15054300	-4.91428800
H	1.27222300	1.12194400	-5.69816800
H	1.43774500	5.02147100	-3.88467900
H	2.76419600	5.37118200	-1.87668900
H	0.60478600	3.52815600	-5.67625700
C	0.32991100	-3.54173600	2.28970600
C	-0.36608900	-2.64988000	3.14043500
C	-0.38178400	-4.50233900	1.53107700
C	0.29728600	-1.63609500	3.90544500
C	-1.80484400	-2.73870100	3.24866000
C	-1.82050000	-4.57958600	1.64492000
C	-0.39988400	-0.79022300	4.72863800
H	1.37030900	-1.52959200	3.80554500
C	-2.49405200	-1.84224600	4.12651300
C	-2.49140200	-3.70125600	2.50218000
C	-1.81608500	-0.89678100	4.84781900
H	0.13034000	-0.02179600	5.28524100
H	-3.57503700	-1.93440800	4.21149100
H	-3.57269900	-3.78155000	2.60276000

H	-2.35246400	-0.22231200	5.50998400
C	5.80195600	2.96601400	1.02317900
H	6.50994500	2.62476600	1.77366200
C	5.37010800	2.10128400	0.05211800
H	5.74810200	1.08575000	0.03601700
C	5.33579700	4.31033000	1.06043400
H	5.68737200	4.98118100	1.83986700
C	4.45691500	4.75203600	0.10888900
H	4.09519000	5.77669400	0.11818100
C	-0.44534100	-6.37419500	-0.03949300
H	0.07406900	-7.07214300	-0.69049400
C	-1.86290300	-6.44487700	0.07524000
H	-2.41212500	-7.19696100	-0.48511500
C	-2.52694200	-5.57194000	0.89520600
H	-3.60897500	-5.61857300	0.99406200
C	0.26731700	-5.43989700	0.66525300
H	1.34661800	-5.40503000	0.57316500
N	1.30317900	-0.72686500	-1.58920700
S	-0.15455500	-0.99995600	-2.10929300
O	-0.62106800	0.02429400	-3.05609600
O	-1.12410500	-1.40654900	-1.05010300
C	0.02339800	-2.54047100	-3.15053700
F	0.94242800	-2.34834200	-4.10427900
F	-1.14840900	-2.82697500	-3.73666200
F	0.39008300	-3.57950800	-2.39447400
C	-5.37669500	-0.47584700	-0.46745600
C	-5.70128000	0.87360000	-1.19554400
H	-6.22605700	1.49359000	-0.46990600
H	-6.42556500	0.66341000	-1.99512500
C	-4.59533200	1.66167900	-1.83822700
C	-4.31282900	-0.22376000	0.63361100
H	-4.72435000	0.49378200	1.34025100
H	-4.13383900	-1.15667800	1.18010100
N	-3.00212700	0.30530000	0.22861300
C	-2.40647100	1.36731000	0.82405900
N	-1.06581000	1.36773300	0.90891500
C	-0.26436400	2.47986900	1.30846600
C	-0.27982600	3.67666300	0.59244700
C	0.58774000	2.32551000	2.40229900
C	0.52746200	4.73570900	1.00311100
C	1.39959700	3.38949800	2.79635300
H	0.61510300	1.37879300	2.92695400
C	1.36779900	4.60201300	2.10927300
H	1.99830900	5.42497100	2.42258300

C	2. 35314800	3. 20532700	3. 94805900
C	0. 44755200	6. 05005600	0. 27560600
F	1. 85773000	2. 34979300	4. 87407900
F	3. 54045000	2. 70693900	3. 54716500
F	2. 60678600	4. 37588300	4. 57695000
F	-0. 46988400	6. 87619000	0. 82990500
F	1. 62760500	6. 71479300	0. 29379700
F	0. 09579200	5. 89090800	-1. 02127900
S	-3. 35281700	2. 71698700	1. 37412300
H	-0. 90774300	3. 77752900	-0. 28320100
H	-0. 52408300	0. 48555700	0. 83166700
H	-2. 35793900	-0. 35559800	-0. 23353900
C	-4. 40213100	3. 01873500	-1. 49078800
H	-3. 94891200	2. 78986200	-0. 29826000
C	-6. 70217800	-0. 94551400	0. 27799800
H	-6. 45527400	-1. 90552000	0. 74905100
H	-7. 42307200	-1. 18779100	-0. 50528200
C	-5. 04391100	-1. 62993700	-1. 43397000
C	-4. 00039800	-2. 53404000	-1. 20254400
C	-5. 86786600	-1. 86828400	-2. 55130500
C	-3. 76227200	-3. 60672500	-2. 06713200
H	-3. 33274200	-2. 41899900	-0. 35866900
C	-5. 64163600	-2. 94100000	-3. 41015200
H	-6. 70626800	-1. 21012600	-2. 76539100
C	-4. 57934000	-3. 81602800	-3. 17400800
H	-2. 92515800	-4. 26650300	-1. 86465600
H	-6. 29542300	-3. 08998300	-4. 26561800
H	-4. 39134800	-4. 64668400	-3. 84857200
C	-7. 33797900	-0. 04000400	1. 32308600
C	-8. 38606600	0. 77361200	1. 06147400
C	-9. 02690400	1. 63930100	2. 12549600
H	-10. 01357100	1. 24301100	2. 40720000
H	-8. 43049700	1. 72873100	3. 03486200
H	-9. 20206900	2. 65318200	1. 74184500
C	-3. 32669100	3. 81327000	-2. 22942000
H	-3. 08210000	4. 72383200	-1. 67346300
H	-2. 40306200	3. 24661100	-2. 37244200
H	-3. 68185300	4. 12201300	-3. 22150900
C	-3. 73981500	1. 02001300	-2. 88532700
H	-4. 01165000	-0. 01721200	-3. 06836900
H	-3. 84494500	1. 58709200	-3. 82209100
H	-2. 66903300	1. 03754700	-2. 65062000
C	-6. 78803900	-0. 16485100	2. 74096900
H	-6. 08528300	-0. 99933200	2. 81907400

H	-6.25519500	0.73541200	3.07381400
H	-7.58607100	-0.35163300	3.46822900
C	-5.58031400	3.91315900	-1.06425400
H	-6.30086900	3.41800200	-0.41203700
H	-5.19434800	4.78530100	-0.52756100
H	-6.10985300	4.27350500	-1.95457700
C	-9.07698600	0.90979500	-0.27733100
H	-8.92729300	1.91456800	-0.69794500
H	-8.75118800	0.18625700	-1.02674300
H	-10.16203800	0.79134200	-0.15281100

TS-EF-7SS-6

l imaginary frequency

H = -5472.478157

G = -5472.691745

E(M06-2X-DCM) = -5473.458901

O	2.34576500	-1.70029200	-0.38889000
O	1.87275400	0.52427300	-1.64756300
P	1.22234300	-0.52850800	-0.55790400
O	0.95618400	0.27421700	0.67904000
C	6.36459700	-0.93226800	0.51047500
C	5.88445000	-0.76714100	-0.78370600
C	4.55542300	-1.08685000	-1.10500300
C	4.14670300	-1.68056400	1.23074500
C	5.50388700	-1.41840000	1.49147700
C	2.00854800	0.12096400	-2.97677700
C	3.07196800	-0.70060400	-3.34166400
C	3.08671500	-1.27353200	-4.62370500
C	2.12966100	-0.92193000	-5.56835500
C	1.15814100	0.01980100	-5.22791600
C	1.06583000	0.55065000	-3.93157500
H	5.87585700	-1.59267300	2.49644300
H	0.43367100	0.34268000	-5.96983300
C	4.37210900	-1.04004300	-2.62074800
C	5.48177600	0.00098600	-2.99891100
H	5.08339600	1.01050300	-2.84202200
H	5.78691300	-0.07624300	-4.04670100
H	5.02832200	-1.86851400	-5.39515800
H	3.90687700	-3.21009500	-5.19185000
C	3.68171800	-1.46443200	-0.08323700
H	7.39903500	-0.70304700	0.75430800
H	2.14049100	-1.36051100	-6.56293200
C	6.62685000	-0.26696900	-2.00246500
H	7.22644700	0.62655000	-1.79282800

H	7. 32105900	-1. 02823900	-2. 38526900
C	4. 22837600	-2. 25959600	-4. 75097700
C	4. 70244000	-2. 41678200	-3. 28829100
H	4. 11235400	-3. 19531500	-2. 79442700
H	5. 76010700	-2. 68382500	-3. 19903900
C	0. 04268300	1. 60472300	-3. 64669500
C	-1. 34017100	1. 30271200	-3. 69832600
C	0. 47189000	2. 94134500	-3. 44254700
C	-1. 83478700	-0. 03040200	-3. 87250100
C	-2. 31016300	2. 36707500	-3. 55544200
C	-0. 50915800	3. 99067600	-3. 28094000
C	-3. 17942500	-0. 28765600	-3. 93217400
H	-1. 12989300	-0. 84989200	-3. 91920400
C	-3. 70433600	2. 05673100	-3. 63728700
C	-1. 86989600	3. 67616000	-3. 34441400
C	-4. 12977800	0. 76931500	-3. 83014600
H	-3. 52697300	-1. 31156700	-4. 02321900
H	-4. 41942400	2. 87103800	-3. 54341700
H	-2. 60423900	4. 47311900	-3. 24177900
H	-5. 19052700	0. 54132300	-3. 88110300
C	3. 30186800	-2. 21848800	2. 34192700
C	3. 16729800	-1. 47155500	3. 54086400
C	2. 75052800	-3. 52270000	2. 25353600
C	3. 67715200	-0. 14011300	3. 69454900
C	2. 49396100	-2. 05831400	4. 67826400
C	2. 03049000	-4. 07134700	3. 38109800
C	3. 59902100	0. 52541100	4. 89097100
H	4. 12321700	0. 35218000	2. 83854500
C	2. 43169800	-1. 32995700	5. 90848700
C	1. 93060400	-3. 33122500	4. 56171700
C	2. 98307900	-0. 08105900	6. 02306200
H	3. 99634400	1. 53359900	4. 97073600
H	1. 94398800	-1. 80179300	6. 75888700
H	1. 41629000	-3. 76522800	5. 41718400
H	2. 94453500	0. 45295100	6. 96930800
C	2. 23658500	4. 62638800	-3. 24185900
H	3. 29239400	4. 88405600	-3. 24081900
C	1. 85325000	3. 32316300	-3. 42612900
H	2. 60773900	2. 56040600	-3. 57944700
C	1. 26473300	5. 65256100	-3. 06857100
H	1. 58538200	6. 68256200	-2. 93625000
C	-0. 06767400	5. 33809700	-3. 09184100
H	-0. 82136900	6. 11347000	-2. 98111500
C	2. 34746500	-5. 60929800	1. 04793100

H	2.46544900	-6.21096400	0.15116400
C	1.60909000	-6.12843400	2.14766600
H	1.16827000	-7.11919800	2.08129800
C	1.46287700	-5.37997500	3.28279700
H	0.91306000	-5.76703900	4.13746300
C	2.90118000	-4.35815600	1.10147900
H	3.46076800	-3.98893100	0.25169000
N	-0.04955400	-1.22180100	-1.27285200
S	-0.56727300	-2.73754900	-1.22515100
O	-1.91415500	-2.78039900	-1.80874700
O	-0.32445100	-3.42741800	0.04966900
C	0.45524500	-3.67642700	-2.48908900
F	0.48083800	-3.01783300	-3.65747900
F	-0.10092000	-4.87628900	-2.68724500
F	1.72049800	-3.86197100	-2.08043500
C	-0.33952100	3.94238600	2.48401100
C	-0.75456200	3.35148300	3.88788200
H	-1.64598000	3.88920800	4.20797500
H	0.02872800	3.61664100	4.61086800
C	-0.97997900	1.87489700	4.04266800
C	-1.27677500	3.38060700	1.38627900
H	-2.29883900	3.68420900	1.61269700
H	-1.01475500	3.83390600	0.42494300
N	-1.29662700	1.92040600	1.21939300
C	-2.41970000	1.17862600	1.10981700
N	-2.34857800	0.01954600	0.43612300
C	-3.40853600	-0.94765400	0.36651300
C	-3.33784300	-2.10558600	1.13824700
C	-4.45401500	-0.75438000	-0.53156800
C	-4.33907200	-3.06928000	1.01746800
C	-5.44134300	-1.73176800	-0.65486600
H	-4.48114600	0.14089500	-1.14133200
C	-5.39155100	-2.88930800	0.12033400
H	-6.15849800	-3.64798700	0.01979100
C	-6.52080500	-1.55295100	-1.68852800
C	-4.31845700	-4.28723200	1.90351700
F	-6.08579500	-1.88415400	-2.92936800
F	-7.60286100	-2.31742300	-1.43280100
F	-6.93664900	-0.26699400	-1.75920600
F	-5.03371000	-4.07578500	3.03820200
F	-4.86668000	-5.36003700	1.29403800
F	-3.07053600	-4.61818000	2.28316100
S	-3.87997400	1.63302100	1.93911400
H	-2.49356100	-2.27095600	1.79728900

H	-1.50784200	-0.20955500	-0.11312800
H	-0.42461000	1.45654600	0.90702200
C	-2.22240400	1.38662000	4.50481200
H	-2.86252500	1.54152300	3.37109900
C	-0.66239000	5.48998900	2.60854300
H	0.00486500	5.88680800	3.38497500
H	-1.67460800	5.56924100	3.01273000
C	1.16088600	3.76280400	2.18161000
C	2.12045800	4.11305700	3.15072200
C	1.63634600	3.33791200	0.93471600
C	3.48632600	4.03458500	2.88828100
H	1.80704000	4.47119000	4.12817600
C	3.00507200	3.24792300	0.66798700
H	0.95720500	3.06065200	0.13840100
C	3.93773800	3.59608900	1.64069200
H	4.19774100	4.32089200	3.65885500
H	3.32352500	2.89391700	-0.30732400
H	5.00234400	3.52791600	1.43439500
C	-0.53917400	6.37070300	1.37612700
C	-1.61452400	6.83476900	0.70062300
C	-1.48182100	7.77277900	-0.48091100
H	-0.47745100	7.79986800	-0.90575800
H	-2.17545800	7.48274800	-1.28084400
H	-1.75619800	8.79910900	-0.19447800
C	-2.35192600	-0.09954000	4.83869900
H	-3.40769000	-0.37906200	4.90016000
H	-1.88039500	-0.74633100	4.09592900
H	-1.89145600	-0.31937900	5.81051100
C	0.87344500	6.79034000	0.99089800
H	1.22146600	6.28709000	0.08043000
H	0.94098500	7.86965100	0.81512200
H	1.58760100	6.54291500	1.77961900
C	0.16060200	0.94845300	3.76900000
H	0.55719900	0.59538100	4.73382000
H	-0.13347100	0.05439800	3.21495600
H	0.97326800	1.42151600	3.22311900
C	-3.15787300	2.24493800	5.37378400
H	-3.26800900	3.27442400	5.02937400
H	-4.15576500	1.79612400	5.37580500
H	-2.79805000	2.26427200	6.40967600
C	-3.06241800	6.52906300	1.01564500
H	-3.51071000	5.91591300	0.22111900
H	-3.22559300	6.00599500	1.95975800
H	-3.64533600	7.45973900	1.04973200

TS-EF-7SR

l imaginary frequency

H = -5472.477823

G = -5472.690900

E(M06-2X-DCM) = -5473.457032

O	-0.44625000	2.94423600	-0.04446000
O	-1.46006300	1.14280500	-1.63210500
P	-0.40845000	1.35339800	-0.38753400
O	-0.92807100	0.45596700	0.69998200
C	-4.01822100	4.87383900	0.95453100
C	-3.70910700	4.60142600	-0.37416100
C	-2.47756800	4.02314300	-0.71939200
C	-1.87234400	3.92225400	1.64886300
C	-3.08501200	4.56812400	1.94521600
C	-1.19681300	1.72659900	-2.87014600
C	-1.46868700	3.08017600	-3.05883500
C	-1.02698400	3.70608500	-4.23586300
C	-0.44312800	2.96590200	-5.25765000
C	-0.30959300	1.58576400	-5.10351500
C	-0.66761400	0.93696400	-3.91098500
H	-3.29421200	4.82145300	2.98036600
H	0.10245500	0.98844000	-5.91159200
C	-2.29214100	4.06880200	-2.23483300
C	-3.79130300	4.05041900	-2.69170300
H	-4.14411500	3.01245600	-2.69212900
H	-3.92502400	4.44809500	-3.70222800
H	-2.10777300	5.49476400	-4.82442300
H	-0.40337200	5.77954100	-4.48750900
C	-1.61542300	3.61588200	0.29688600
H	-4.96502300	5.33698000	1.22114900
H	-0.10508300	3.44836000	-6.17122300
C	-4.54327900	4.85533000	-1.61056400
H	-5.58370600	4.53221000	-1.48931100
H	-4.57335300	5.92612000	-1.85637700
C	-1.27610200	5.19748800	-4.17028300
C	-1.62238400	5.41230400	-2.68060000
H	-0.69884100	5.54652300	-2.10698900
H	-2.26335700	6.28114800	-2.50135500
C	-0.54596600	-0.55424300	-3.82750800
C	0.72641900	-1.17684100	-3.86022900
C	-1.72310300	-1.34584000	-3.83456100
C	1.95127700	-0.43568500	-3.84068900
C	0.81746400	-2.62055300	-3.90203500

C	-1.61606600	-2.78818800	-3.85852300
C	3.16670400	-1.06664200	-3.88086400
H	1.91023500	0.64169700	-3.75703200
C	2.10651400	-3.23921500	-3.95613500
C	-0.35199500	-3.38451900	-3.89151700
C	3.25085800	-2.48660100	-3.95219500
H	4.07639700	-0.47690500	-3.82928500
H	2.15446100	-4.32504300	-4.00125700
H	-0.27744200	-4.46989500	-3.92707100
H	4.22569300	-2.96488800	-3.97634300
C	-0.88979900	3.64131500	2.74217400
C	-1.23900900	2.78044800	3.81315100
C	0.36512900	4.30252900	2.74511600
C	-2.49665400	2.09823900	3.89032700
C	-0.30241300	2.56680700	4.89438000
C	1.30203300	4.05380300	3.81697900
C	-2.82157300	1.30615900	4.96213000
H	-3.20723500	2.22342000	3.08253200
C	-0.67535600	1.72512000	5.98955000
C	0.94485000	3.19435800	4.85833600
C	-1.90253300	1.11795400	6.03402600
H	-3.79198700	0.81753600	4.99598900
H	0.03980300	1.59017300	6.79803400
H	1.65034900	3.02146600	5.66868900
H	-2.17981500	0.49731000	6.88238500
C	-4.15902900	-1.57448700	-3.89127800
H	-5.14393200	-1.11619400	-3.91617800
C	-3.04027500	-0.78306800	-3.86012200
H	-3.14768000	0.29536800	-3.86760400
C	-4.04671300	-2.99430000	-3.89818000
H	-4.94393200	-3.60641000	-3.92939400
C	-2.80860400	-3.57897900	-3.88077900
H	-2.70612600	-4.66178200	-3.90461100
C	1.97080000	5.86743500	1.77457500
H	2.23585400	6.57523000	0.99399000
C	2.90196100	5.59135600	2.81437900
H	3.87047300	6.08361500	2.81543400
C	2.57082000	4.71235400	3.80812700
H	3.26660600	4.49782100	4.61566900
C	0.74959300	5.24868900	1.74275800
H	0.05505400	5.48111900	0.94468300
N	1.07913500	1.06060500	-0.94709900
S	2.44730600	1.84845800	-0.64512000
O	3.55327400	1.04397300	-1.17970500

O	2. 55598200	2. 38515600	0. 71768400
C	2. 44486000	3. 35769400	-1. 76891900
F	2. 08933500	3. 01853600	-3. 01841900
F	3. 68105700	3. 86524300	-1. 80010500
F	1. 60662800	4. 31050500	-1. 33896500
C	-2. 72455000	-2. 93136000	1. 13857600
C	-2. 35137800	-2. 39412600	2. 59061800
H	-3. 02909800	-2. 86183400	3. 31234100
H	-2. 56306600	-1. 32634800	2. 60755000
C	-0. 95720600	-2. 54690600	3. 16591100
C	-1. 43550400	-3. 26143500	0. 33263800
H	-1. 05275900	-4. 24318900	0. 60540600
H	-1. 68239600	-3. 28948400	-0. 73549700
N	-0. 33796600	-2. 30946000	0. 51358800
C	0. 96822500	-2. 65298600	0. 53729400
N	1. 86503100	-1. 70945400	0. 19822800
C	3. 28550700	-1. 83830700	0. 33765400
C	3. 96142700	-0. 99609600	1. 21995300
C	3. 98742100	-2. 75283700	-0. 44499500
C	5. 34903200	-1. 09072400	1. 33061900
C	5. 37469100	-2. 83728300	-0. 32643900
H	3. 45612000	-3. 37676400	-1. 15300800
C	6. 06130000	-2. 01140100	0. 56278300
H	7. 13924800	-2. 07722300	0. 64959700
C	6. 12980200	-3. 78089100	-1. 22390400
C	6. 07848000	-0. 23717700	2. 33547500
F	6. 34137400	-3. 24199000	-2. 45145600
F	7. 34156300	-4. 09799500	-0. 72171100
F	5. 45279200	-4. 93343800	-1. 42042200
F	6. 17601200	-0. 86948500	3. 53257000
F	7. 33994900	0. 03630700	1. 93694000
F	5. 45101200	0. 93131900	2. 55786700
S	1. 46321300	-4. 21523900	1. 10773600
H	3. 41544800	-0. 25277600	1. 79052200
H	1. 53355300	-0. 82608700	-0. 22194600
H	-0. 55823900	-1. 30529900	0. 39619900
C	-0. 38411400	-3. 78427100	3. 52571200
H	0. 31871100	-3. 95021300	2. 43447200
C	-0. 24215200	-1. 26421100	3. 46222800
H	0. 84439000	-1. 37814300	3. 48044200
H	-0. 51193000	-0. 47122100	2. 76181900
H	-0. 53909200	-0. 92387400	4. 46778800
C	-3. 62476400	-4. 18421500	1. 19254600
C	-4. 68355900	-4. 27555600	2. 11370000

C	-3.48307800	-5.24211700	0.27786900
C	-5.53663000	-5.37831500	2.14157000
H	-4.86360300	-3.47077100	2.81837900
C	-4.33567000	-6.34827200	0.30133100
H	-2.70454700	-5.22088700	-0.47630800
C	-5.36564200	-6.42629900	1.23618300
H	-6.33903900	-5.41406200	2.87389100
H	-4.18730700	-7.14974400	-0.41749800
H	-6.02683900	-7.28813100	1.25865800
C	-3.49740400	-1.80606400	0.32684700
H	-3.61927000	-2.20543100	-0.68295700
H	-2.81912800	-0.94995900	0.23848100
C	-4.83394400	-1.29722900	0.84627100
C	-6.02599500	-1.74172400	0.38815600
C	-4.74345100	-0.17783300	1.87357800
H	-4.79767200	-0.54360600	2.90976300
H	-3.79415300	0.35626900	1.77228600
H	-5.53992200	0.56227800	1.75656600
C	-7.35398400	-1.22663200	0.90236000
H	-7.89866400	-0.69173100	0.11070000
H	-7.99478100	-2.06927000	1.19691500
H	-7.27268000	-0.56159400	1.76333400
C	0.74922300	-3.81919400	4.56229600
H	0.34673900	-3.65382000	5.56944500
H	1.22420400	-4.80487100	4.54984000
H	1.52962900	-3.07839300	4.38132400
C	-6.21425900	-2.79681900	-0.67745600
H	-6.91137200	-2.43218600	-1.44535300
H	-5.29492200	-3.09982700	-1.17797300
H	-6.66770800	-3.70046500	-0.24793600
C	-1.23962000	-5.04937200	3.58385000
H	-1.71121900	-5.13573500	4.57174500
H	-2.02699900	-5.07944400	2.83162500
H	-0.60856900	-5.93401300	3.44664000

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l imaginary frequency

H = -5472.476124

G = -5472.690863

E(M06-2X-DCM) = -5473.455592

O	1.25125600	-2.53512400	0.86639200
O	1.49590200	-1.57073600	-1.54493600
P	0.74501400	-1.32410000	-0.10380700
O	1.17533000	0.04071300	0.35486700

C	5. 31409700	-3. 30348100	1. 53380900
C	4. 69216400	-3. 73557500	0. 36775800
C	3. 31551100	-3. 54177200	0. 17508300
C	3. 18099000	-2. 39953200	2. 32987600
C	4. 54808100	-2. 67617200	2. 51383800
C	1. 16766700	-2. 69441700	-2. 30851500
C	1. 68602300	-3. 93953400	-1. 95544300
C	1. 18993500	-5. 09292700	-2. 58465300
C	0. 28985900	-4. 99490100	-3. 63893600
C	-0. 09339800	-3. 72908900	-4. 08124500
C	0. 32651300	-2. 55743500	-3. 43112300
H	5. 01068000	-2. 37725300	3. 44956400
H	-0. 74840500	-3. 63140500	-4. 94207100
C	2. 85365600	-4. 32258100	-1. 05117300
C	4. 18660100	-4. 35044600	-1. 87612200
H	4. 27885700	-3. 40482800	-2. 42299400
H	4. 20691100	-5. 16254000	-2. 60899400
H	2. 50122800	-6. 82293100	-2. 61107400
H	1. 00136200	-7. 08802600	-1. 72856900
C	2. 59332100	-2. 80666600	1. 11470400
H	6. 37707900	-3. 46732200	1. 69211200
H	-0. 09578200	-5. 88569600	-4. 12821600
C	5. 30339900	-4. 44950400	-0. 81704000
H	6. 24242400	-3. 98956600	-1. 14603700
H	5. 53409900	-5. 49614700	-0. 57349900
C	1. 76981000	-6. 33833900	-1. 94926600
C	2. 43954400	-5. 78392100	-0. 67273000
H	1. 70303900	-5. 73919900	0. 13644800
H	3. 28707500	-6. 38452500	-0. 32788800
C	-0. 04729300	-1. 23690800	-4. 03246800
C	-1. 38746200	-0. 78346100	-4. 00881600
C	0. 93407000	-0. 51950200	-4. 76343200
C	-2. 42359200	-1. 47394600	-3. 30090400
C	-1. 74763500	0. 42038800	-4. 72627800
C	0. 56425200	0. 69459500	-5. 45610200
C	-3. 71883900	-1. 02762900	-3. 32518100
H	-2. 16798600	-2. 34928900	-2. 71856900
C	-3. 11275100	0. 84784900	-4. 72973000
C	-0. 76278100	1. 13175800	-5. 41586700
C	-4. 07509800	0. 14025400	-4. 06010500
H	-4. 47766300	-1. 55755700	-2. 75799900
H	-3. 36951100	1. 74600500	-5. 28713300
H	-1. 04020700	2. 03602200	-5. 95451900
H	-5. 10912100	0. 47087300	-4. 07026900

C	2. 42893200	-1. 75609700	3. 45160400
C	2. 84223700	-0. 48863300	3. 93650200
C	1. 39552900	-2. 46590200	4. 11618600
C	3. 85690500	0. 29786200	3. 29815000
C	2. 23191100	0. 05716900	5. 12867300
C	0. 75886500	-1. 88156400	5. 27550800
C	4. 27799500	1. 49260100	3. 82575800
H	4. 29516100	-0. 06531500	2. 37602400
C	2. 70057100	1. 30653700	5. 64696500
C	1. 20079500	-0. 64629100	5. 75606800
C	3. 70225400	2. 00288000	5. 02500500
H	5. 06064800	2. 05653900	3. 32439600
H	2. 24544700	1. 68587900	6. 55951200
H	0. 73916600	-0. 22930600	6. 64924300
H	4. 05827500	2. 94292100	5. 43863200
C	3. 20792000	-0. 26503700	-5. 63222200
H	4. 22579100	-0. 63576100	-5. 72057800
C	2. 28901300	-0. 96670600	-4. 89502700
H	2. 58421700	-1. 88941300	-4. 40866700
C	2. 84272100	0. 94342900	-6. 29139700
H	3. 58330000	1. 48622800	-6. 87277900
C	1. 55696100	1. 40541800	-6. 20157400
H	1. 25895000	2. 31842600	-6. 71228600
C	-0. 04430000	-4. 42250600	4. 37658600
H	-0. 36015000	-5. 40513300	4. 03784100
C	-0. 68998800	-3. 82633200	5. 49541100
H	-1. 49367800	-4. 35606800	5. 99914700
C	-0. 29166500	-2. 59367000	5. 93374700
H	-0. 76540100	-2. 12993700	6. 79573300
C	0. 96336800	-3. 77044300	3. 71742000
H	1. 44218200	-4. 24909300	2. 87292800
N	-0. 83424800	-1. 56408400	-0. 33636700
S	-1. 91292200	-2. 30350900	0. 58942500
O	-3. 24530500	-2. 03593300	0. 03184100
O	-1. 70342500	-2. 12667300	2. 03394600
C	-1. 70621500	-4. 14507100	0. 27997300
F	-1. 66533200	-4. 39509500	-1. 03668100
F	-2. 75471100	-4. 78615100	0. 80602900
F	-0. 58935100	-4. 63460000	0. 83899400
C	1. 98507500	3. 83648500	0. 35938200
C	1. 70481100	3. 65771800	1. 92543600
H	2. 11318900	4. 53088200	2. 44039000
H	2. 28401700	2. 79377900	2. 25909500
C	0. 30773900	3. 46741300	2. 45930200

C	0.68907900	3.63894200	-0.47121400
H	0.06059800	4.52469200	-0.40028000
H	0.95792200	3.51669900	-1.52348100
N	-0.14179300	2.49622700	-0.08118300
C	-1.49085900	2.51007500	-0.06048200
N	-2.13667700	1.32760800	-0.08647100
C	-3.54406900	1.18056400	0.16057500
C	-3.96998900	0.62943600	1.36749200
C	-4.46747800	1.54831900	-0.81587200
C	-5.33571400	0.46839000	1.60467000
C	-5.82985600	1.37900300	-0.56927400
H	-4.12259700	1.94989500	-1.76071100
C	-6.27018600	0.84451000	0.64193200
H	-7.32953400	0.71434000	0.82918000
C	-6.82811000	1.70608100	-1.64701300
C	-5.80249200	-0.05706500	2.93726800
F	-7.05861000	0.63820600	-2.45336800
F	-8.02269500	2.07095200	-1.13501400
F	-6.40008800	2.70824700	-2.44483500
F	-5.95548700	0.95205400	3.83243900
F	-6.99878700	-0.67653400	2.84087600
F	-4.92670200	-0.92631300	3.47244900
S	-2.37163700	3.99574200	0.11666200
H	-3.24398600	0.29491800	2.10041500
H	-1.61319400	0.45637600	-0.25220900
H	0.32171100	1.56962100	-0.03627300
C	-0.61263300	4.53228700	2.57171000
H	-1.26934600	4.29809200	1.48112700
C	-0.01336800	2.10631500	2.99392200
H	-1.08290500	1.88444300	2.99254700
H	0.52097200	1.31763000	2.45961700
H	0.31882300	2.06492100	4.04316800
C	2.55780600	5.24281500	0.06586800
C	3.54086300	5.79859500	0.90415300
C	2.18214100	5.99515700	-1.05868700
C	4.09785100	7.05128700	0.65366600
H	3.89616300	5.24334700	1.76791600
C	2.73987000	7.25007300	-1.31714600
H	1.44691400	5.61620200	-1.75889900
C	3.69657500	7.78945900	-0.46055400
H	4.85096500	7.44692300	1.33010500
H	2.41832300	7.80321600	-2.19556800
H	4.12645100	8.76738900	-0.65846300
C	3.09246900	2.76326600	-0.00298500

H	2.69436800	1.77904800	0.26889100
H	3.92667000	2.95246400	0.67850700
C	3.57900900	2.70610200	-1.44234100
C	4.74451500	3.24491800	-1.86328200
C	2.70162200	1.90294700	-2.39460200
H	3.28496000	1.19117300	-2.98530300
H	1.96739100	1.30739100	-1.84835700
H	2.15815500	2.52877400	-3.11580100
C	5.20211400	3.15934800	-3.30405300
H	5.48962200	4.15528000	-3.66913000
H	6.10063700	2.53052300	-3.39114700
H	4.44716200	2.76160800	-3.98380100
C	-1.75445000	4.43936500	3.59416500
H	-1.37156000	4.62258900	4.60585800
H	-2.50524900	5.20467600	3.37615900
H	-2.26234300	3.47349000	3.59208300
C	5.74776000	3.97145300	-0.99742200
H	5.78697200	5.03879000	-1.25341300
H	5.54889700	3.90202500	0.07283300
H	6.75491100	3.56955700	-1.17731800
C	-0.13903400	5.97274500	2.36530100
H	0.31405200	6.35848900	3.28807900
H	0.59010200	6.07790000	1.56066900
H	-0.99377800	6.61438200	2.12793100

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l imaginary frequency

H = -5472.483368

G = -5472.694891

E(M06-2X-DCM) = -5473.455484

O	1.33079500	-2.90167700	-0.09056800
O	2.94779500	-0.95293800	-0.60229300
P	1.37827600	-1.27199600	-0.27927600
O	0.99905800	-0.52458800	0.95685500
C	3.81349200	-4.65771000	2.78920900
C	4.28073600	-4.40672300	1.50345400
C	3.43295600	-3.86651600	0.52469500
C	1.62635100	-3.75585900	2.16464900
C	2.48961100	-4.35024600	3.10052600
C	3.51018500	-1.42216100	-1.78965900
C	3.90219400	-2.75488200	-1.89093000
C	4.25574800	-3.26557800	-3.14990900
C	4.35198200	-2.42515700	-4.25423100
C	4.10606200	-1.06002000	-4.09234100

C	3.66947300	-0.52974800	-2.86818700
H	2.10801100	-4.55035200	4.09757700
H	4.23088200	-0.38396600	-4.93330200
C	4.14669500	-3.81868200	-0.82295500
C	5.63827200	-3.76026700	-0.33858400
H	5.88656000	-2.72064200	-0.09563500
H	6.34011500	-4.09972500	-1.10646400
H	5.54566800	-5.01334500	-3.15153800
H	3.96707800	-5.30294400	-3.87333600
C	2.13281800	-3.50532600	0.87459700
H	4.46839100	-5.08167800	3.54629800
H	4.63240600	-2.81688000	-5.22888100
C	5.67172300	-4.61197100	0.94693600
H	6.45621800	-4.29688600	1.64434100
H	5.85717100	-5.67165600	0.72039000
C	4.47899000	-4.76179900	-3.06920500
C	3.92281000	-5.11403800	-1.66960100
H	2.84655700	-5.31022400	-1.73546400
H	4.39777400	-5.99349900	-1.22286600
C	3.45374200	0.94317300	-2.71263000
C	2.42374400	1.60530800	-3.42393300
C	4.33951300	1.68578500	-1.88992800
C	1.49548900	0.91500300	-4.26788300
C	2.27411200	3.03842100	-3.29461200
C	4.16062600	3.11302700	-1.75121300
C	0.52354800	1.58802200	-4.96000600
H	1.55093300	-0.16456900	-4.33016600
C	1.24488500	3.70296600	-4.03371100
C	3.13323500	3.74943100	-2.45324600
C	0.39947300	3.00239000	-4.85229300
H	-0.17593600	1.03371700	-5.57860800
H	1.16096600	4.78352300	-3.93820900
H	2.99796400	4.82240000	-2.33785400
H	-0.36926200	3.52061300	-5.42082100
C	0.22307600	-3.43417500	2.57424400
C	-0.01265800	-2.43263900	3.54740700
C	-0.85619700	-4.18952000	2.05471600
C	1.03124700	-1.61330800	4.08920300
C	-1.35868300	-2.19831700	4.01961600
C	-2.19936700	-3.93117300	2.52146400
C	0.77325000	-0.66515900	5.04595400
H	2.04083600	-1.73593700	3.71556900
C	-1.58476700	-1.20170100	5.02116100
C	-2.41278100	-2.94904200	3.49244100

C	-0.55232900	-0.45956500	5.52671300
H	1.58271300	-0.04925800	5.42762600
H	-2.60288400	-1.04764900	5.37208600
H	-3.42386500	-2.77195300	3.85545100
H	-0.73775200	0.29417500	6.28729000
C	6.27610500	1.83493700	-0.40263300
H	7.10311500	1.35298200	0.11207100
C	5.43995800	1.09024600	-1.19266200
H	5.61639000	0.02669100	-1.30353200
C	6.07522500	3.23547400	-0.24759700
H	6.74369100	3.80903000	0.38900700
C	5.04789300	3.85328100	-0.90794400
H	4.88173800	4.92132000	-0.79839300
C	-1.74210500	-5.95485500	0.61452400
H	-1.57677900	-6.74093000	-0.11732800
C	-3.06495800	-5.68638400	1.06737600
H	-3.89618000	-6.26871200	0.67876700
C	-3.28165400	-4.70449000	1.99624100
H	-4.28548700	-4.49798400	2.36111000
C	-0.67882000	-5.23577800	1.09368800
H	0.32225900	-5.45930500	0.74329600
N	0.58583000	-1.01536600	-1.67348400
S	-0.97483300	-1.07921100	-1.82883100
O	-1.47390600	-0.11076100	-2.82226700
O	-1.73172200	-1.13623700	-0.54330100
C	-1.32048600	-2.73535500	-2.62463400
F	-0.69202600	-2.81390800	-3.80279800
F	-2.64021500	-2.86017300	-2.83276300
F	-0.90968000	-3.73528800	-1.84341900
C	-5.06129400	1.13260100	-0.13055000
C	-5.12156100	2.54615800	-0.82640700
H	-5.50735200	3.23625900	-0.07879600
H	-5.87060900	2.49242700	-1.62738600
C	-3.90044600	3.15578900	-1.45039100
C	-3.99517800	1.20265500	1.01140000
H	-4.23420000	2.02679700	1.68475400
H	-4.05302200	0.27520700	1.58982100
N	-2.59703200	1.35415300	0.59008400
C	-1.71198200	2.19819300	1.17969500
N	-0.41778400	1.82748400	1.16980700
C	0.69059800	2.61649500	1.59449000
C	0.94288300	3.88532200	1.06840100
C	1.58005900	2.04989000	2.50811900
C	2.06367300	4.59685300	1.49243400

C	2. 70486900	2. 76902300	2. 91465300
H	1. 39969900	1. 04777600	2. 87786800
C	2. 95155700	4. 04734200	2. 41959900
H	3. 83059000	4. 59734200	2. 73144300
C	3. 62232900	2. 14883600	3. 93535100
C	2. 28924700	5. 98990200	0. 97103300
F	3. 06988900	2. 17648000	5. 17651100
F	3. 87741800	0. 85251400	3. 66014000
F	4. 80547600	2. 79256600	4. 01740300
F	1. 64996200	6. 91755600	1. 71907800
F	3. 59969500	6. 32677600	0. 96785400
F	1. 83360900	6. 13522300	-0. 29769300
S	-2. 23551900	3. 70731800	1. 84529800
H	0. 27981100	4. 30852100	0. 32589400
H	-0. 15472500	0. 83858400	0. 99134800
H	-2. 19750300	0. 50052100	0. 16882700
C	-3. 38502000	4. 39001400	-0. 94636500
H	-2. 95652900	3. 99842300	0. 14097900
C	-2. 19165300	5. 01839000	-1. 67061900
H	-1. 73969900	5. 78647200	-1. 03552500
H	-1. 41459400	4. 29044000	-1. 91910800
H	-2. 50591000	5. 50803900	-2. 60153300
C	-3. 27722000	2. 51417900	-2. 64566500
H	-3. 99649000	1. 88337500	-3. 17080500
H	-2. 88755200	3. 26499300	-3. 33847300
H	-2. 43427700	1. 85219500	-2. 39586600
C	-4. 35136600	5. 47389700	-0. 41715700
H	-5. 12397600	5. 09156900	0. 25108700
H	-3. 77326500	6. 21393500	0. 14368900
H	-4. 83628100	5. 98480600	-1. 25713000
C	-6. 40504900	0. 85989600	0. 59134800
C	-7. 49894900	1. 73760700	0. 58290200
C	-6. 55208000	-0. 33965500	1. 31275600
C	-8. 67969400	1. 43946100	1. 27001900
H	-7. 46119400	2. 67111100	0. 03301000
C	-7. 72365200	-0. 63750500	2. 00449200
H	-5. 74462900	-1. 06466200	1. 32926500
C	-8. 79766700	0. 25383300	1. 98936000
H	-9. 50583900	2. 14486100	1. 23801800
H	-7. 79751100	-1. 57319800	2. 55230800
H	-9. 71325000	0. 02341000	2. 52685700
C	-4. 72814000	-0. 06568600	-1. 09307000
H	-4. 27010300	-0. 83371700	-0. 47398600
H	-3. 92818900	0. 23692200	-1. 77391100

C	-5.86368000	-0.68932100	-1.89630300
C	-6.13579400	-2.01220700	-1.84368000
C	-6.61926200	0.25687600	-2.80774200
H	-7.29907600	0.91420100	-2.24773700
H	-5.92358200	0.90378500	-3.35888300
H	-7.21864600	-0.25849300	-3.55911600
C	-5.36790000	-3.02876400	-1.02265200
H	-5.20075300	-3.93350000	-1.62107500
H	-4.38748500	-2.70097100	-0.67722300
H	-5.95486800	-3.34394700	-0.14731700
C	-7.26445700	-2.67406200	-2.60828000
H	-7.82345800	-3.34055700	-1.93758200
H	-7.98447100	-1.98124600	-3.04603900
H	-6.87078000	-3.30979100	-3.41431400

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l imaginary frequency

H = -5472.479047

G = -5472.691046

E(M06-2X-DCM) = -5473.452750

O	1.08101400	-2.89969000	0.01688000
O	3.07217600	-1.25038700	-0.03611000
P	1.44138200	-1.29727500	-0.04501900
O	0.95134100	-0.55564100	1.15825100
C	2.49640000	-5.02834300	3.33635100
C	3.29122200	-4.85679400	2.20797700
C	2.79408600	-4.19499400	1.07529300
C	0.68576000	-3.79976500	2.24012300
C	1.19847600	-4.51927200	3.33315500
C	3.78219800	-1.81689800	-1.09705500
C	3.97769800	-3.19650400	-1.13575200
C	4.51827700	-3.77619500	-2.29442300
C	4.97713200	-2.97965600	-3.33803900
C	4.89997000	-1.59176900	-3.21570300
C	4.29160800	-0.97854300	-2.10823800
H	0.56264100	-4.65478200	4.20329500
H	5.29531700	-0.95650000	-4.00285300
C	3.80527400	-4.27030400	-0.06364800
C	5.13060000	-4.43872800	0.75822100
H	5.47023900	-3.44809900	1.08173800
H	5.93371100	-4.88970000	0.16739700
H	5.50201000	-5.69452600	-2.03219400
H	4.10708700	-5.75978200	-3.10337000
C	1.51888500	-3.63350200	1.11732700

H	2. 87809000	-5. 54568600	4. 21298600
H	5. 40365900	-3. 42593700	-4. 23300000
C	4. 72827800	-5. 27511100	1. 99070500
H	5. 36149200	-5. 07705900	2. 86301700
H	4. 80204400	-6. 35251300	1. 78507000
C	4. 49407200	-5. 28696100	-2. 19332100
C	3. 58580600	-5. 52856400	-0. 96644300
H	2. 53632100	-5. 55641700	-1. 28132800
H	3. 80388300	-6. 46405700	-0. 44118800
C	4. 25183900	0. 51433200	-2. 01528200
C	3. 51975500	1. 27109000	-2. 96315500
C	5. 01820000	1. 17124300	-1. 01881500
C	2. 70785000	0. 67060700	-3. 97861700
C	3. 56238300	2. 71539000	-2. 90884700
C	5. 03376200	2. 61535400	-0. 96637500
C	2. 02211800	1. 43376400	-4. 88626200
H	2. 60814900	-0. 40733700	-3. 99972200
C	2. 82969600	3. 47503200	-3. 87412700
C	4. 31003100	3. 34667900	-1. 91180100
C	2. 08817400	2. 85519400	-4. 84291600
H	1. 39804000	0. 94915500	-5. 63157300
H	2. 87459600	4. 56000300	-3. 81329600
H	4. 32636200	4. 43286000	-1. 86805800
H	1. 53612200	3. 44249300	-5. 57238600
C	-0. 71135300	-3. 26868500	2. 32744600
C	-1. 01396800	-2. 24638500	3. 25993600
C	-1. 74396900	-3. 85647800	1. 55718400
C	-0. 00512300	-1. 56812300	4. 01884900
C	-2. 38688700	-1. 83892600	3. 45588200
C	-3. 11142900	-3. 43109400	1. 75323100
C	-0. 32685400	-0. 58318800	4. 91645800
H	1. 03286200	-1. 82756100	3. 85189600
C	-2. 68206500	-0. 81787200	4. 41488900
C	-3. 39792100	-2. 44750500	2. 70526700
C	-1. 68515300	-0. 20702600	5. 12667500
H	0. 46220100	-0. 07404600	5. 46393100
H	-3. 72228000	-0. 53558900	4. 56222100
H	-4. 43315900	-2. 15200900	2. 86876600
H	-1. 92289200	0. 57020700	5. 84808200
C	6. 53340800	1. 13601300	0. 90153500
H	7. 12188500	0. 57436400	1. 62209900
C	5. 81317800	0. 47025800	-0. 05522700
H	5. 84546100	-0. 61250600	-0. 09035700
C	6. 52223300	2. 55806400	0. 96371600

H	7.09536300	3.06809000	1.73334800
C	5.79773200	3.27296200	0.04901100
H	5.78163400	4.35944600	0.07693700
C	-2.52290800	-5.44380800	-0.13055100
H	-2.30790400	-6.22099000	-0.85882200
C	-3.86741500	-5.01654800	0.06171000
H	-4.66562800	-5.47288000	-0.51766500
C	-4.14930300	-4.04257100	0.98182500
H	-5.17407100	-3.71877200	1.15151400
C	-1.50188900	-4.88884600	0.59535800
H	-0.48560000	-5.23271800	0.44243100
N	1.00259900	-0.82352800	-1.52889200
S	-0.46678500	-0.78081900	-2.08060300
O	-0.69294700	0.35345800	-2.99140400
O	-1.53105700	-1.01604600	-1.06032200
C	-0.56156400	-2.28042800	-3.19435300
F	0.40456300	-2.22227700	-4.11960400
F	-1.74773000	-2.30886300	-3.82236000
F	-0.42247700	-3.40588400	-2.49051600
C	-5.10282900	0.93274500	-0.05735400
C	-5.26002200	2.26550300	-0.89261600
H	-5.67020800	3.02589800	-0.23282900
H	-6.01993400	2.07203200	-1.65721900
C	-4.08138600	2.82341000	-1.63407500
C	-3.93035100	1.05961200	0.97628900
H	-4.12532800	1.89320100	1.64914700
H	-3.92868900	0.14226200	1.57620200
N	-2.56689400	1.23324200	0.45709500
C	-1.69545700	2.15119300	0.94592900
N	-0.40016700	1.80552200	0.99705700
C	0.68392000	2.66226300	1.35104900
C	0.99287300	3.80171200	0.60779000
C	1.48269500	2.28802700	2.43312400
C	2.08331900	4.58719700	0.97862400
C	2.57404300	3.07991800	2.78950700
H	1.24972900	1.38230600	2.98005700
C	2.87543900	4.23687500	2.07303800
H	3.72347100	4.84893900	2.35470200
C	3.46156700	2.65034400	3.92872000
C	2.38379100	5.84893800	0.21560000
F	2.76684400	1.97759300	4.87582500
F	4.45507100	1.83631200	3.51593300
F	4.04440700	3.71123400	4.53260400
F	1.77615200	6.92617300	0.76343800

F	3. 71121000	6. 12243300	0. 19382600
F	1. 96830500	5. 77570300	-1. 06924000
S	-2. 24447200	3. 72562800	1. 42194300
H	0. 39842200	4. 06394200	-0. 25799300
H	-0. 12102700	0. 80265600	0. 96462300
H	-2. 14044200	0. 39225900	0. 04280200
C	-3. 55946400	4. 10194700	-1. 31616500
H	-3. 03576400	3. 80598200	-0. 18603600
C	-2. 41651600	4. 64501800	-2. 17353400
H	-1. 93135400	5. 48163700	-1. 66138300
H	-1. 65398800	3. 88959200	-2. 38134900
H	-2. 78897600	5. 02143600	-3. 13543100
C	-3. 51115900	2. 03635800	-2. 77195000
H	-4. 17322600	1. 21689900	-3. 05573600
H	-3. 36665800	2. 69106700	-3. 64013700
H	-2. 52245200	1. 60538200	-2. 55857200
C	-4. 47477900	5. 22922800	-0. 80148600
H	-5. 21307200	4. 90132700	-0. 06837600
H	-3. 86057900	6. 00003300	-0. 32595900
H	-5. 00455200	5. 69059000	-1. 64338700
C	-6. 33993500	0. 74865300	0. 86162100
C	-6. 76236100	1. 78286400	1. 71544800
C	-7. 01367300	-0. 47956700	0. 95933500
C	-7. 81601200	1. 60638800	2. 61244400
H	-6. 26003800	2. 74627600	1. 70303700
C	-8. 06768900	-0. 66125000	1. 85694100
H	-6. 74288700	-1. 29996300	0. 30522800
C	-8. 47563200	0. 38002900	2. 68913000
H	-8. 11447100	2. 42982100	3. 25571100
H	-8. 57186600	-1. 62312800	1. 89848400
H	-9. 29593100	0. 23883300	3. 38732600
C	-4. 81088000	-0. 30958000	-0. 93650500
H	-4. 71120800	-1. 16385600	-0. 25170300
H	-3. 78914800	-0. 19313400	-1. 31054600
C	-5. 59974300	-0. 81133100	-2. 15414500
C	-6. 79360300	-0. 46749900	-2. 68914100
C	-4. 77584200	-1. 90748300	-2. 82939000
H	-4. 19761500	-1. 51937300	-3. 67811200
H	-4. 04869900	-2. 33617800	-2. 13460400
H	-5. 39884700	-2. 72562500	-3. 20169800
C	-7. 83154300	0. 49965200	-2. 16375700
H	-8. 81069000	0. 00024200	-2. 14196300
H	-7. 65015800	0. 87445500	-1. 16033200
H	-7. 94977700	1. 35606800	-2. 84450300

C	-7.27043700	-1.11977000	-3.98033200
H	-6.45689100	-1.36914900	-4.66562900
H	-7.82852700	-2.04648200	-3.78007100
H	-7.95676600	-0.45118800	-4.51304000

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l imaginary frequency

H = -5472.484439

G = -5472.698151

E(M06-2X-DCM) = -5473.457044

O	1.40530000	-2.91715100	-0.18050600
O	2.92581800	-0.85914500	-0.56281200
P	1.36263400	-1.28349200	-0.33544800
O	0.87778300	-0.58839400	0.89535200
C	3.89389300	-4.61814400	2.72861700
C	4.38748100	-4.29664500	1.46876500
C	3.54256200	-3.77399400	0.47785800
C	1.67565400	-3.84125100	2.04992900
C	2.54232900	-4.40849500	2.99904700
C	3.57336300	-1.24347200	-1.73696800
C	4.03336900	-2.55014500	-1.87720800
C	4.46311700	-2.98887000	-3.13911200
C	4.56619700	-2.09610000	-4.20115500
C	4.25942400	-0.75009300	-3.98868700
C	3.75028400	-0.29434100	-2.76241000
H	2.13785100	-4.67096600	3.97239000
H	4.39608300	-0.03057400	-4.79089200
C	4.29674800	-3.63974200	-0.84153100
C	5.76646800	-3.51693700	-0.30403600
H	5.94900000	-2.47385200	-0.02085300
H	6.51060200	-3.79250800	-1.05751700
H	5.83717600	-4.67108700	-3.16387200
H	4.29901000	-5.00733400	-3.94972600
C	2.21073700	-3.50497500	0.79139800
H	4.54812400	-5.02575400	3.49519500
H	4.90314800	-2.43060000	-5.17919500
C	5.80540200	-4.40608600	0.95521000
H	6.54764700	-4.07094000	1.68860300
H	6.05706900	-5.44624900	0.70341600
C	4.75725100	-4.47494000	-3.10824300
C	4.17397300	-4.91119900	-1.74300000
H	3.11329300	-5.16323200	-1.85464500
H	4.68224700	-5.78023200	-1.31268200
C	3.49801100	1.16499800	-2.54246100

C	2. 48109500	1. 84487700	-3. 25541400
C	4. 34676800	1. 88178100	-1. 65965000
C	1. 58318100	1. 17727800	-4. 14839800
C	2. 31190600	3. 27030800	-3. 07460400
C	4. 15171200	3. 30186500	-1. 47465300
C	0. 61895700	1. 86547500	-4. 83696600
H	1. 65303500	0. 10158200	-4. 24944700
C	1. 29384200	3. 95172600	-3. 81353800
C	3. 14154700	3. 95667600	-2. 18451200
C	0. 47618700	3. 27327700	-4. 67833100
H	-0. 06062900	1. 32602500	-5. 48946500
H	1. 19512200	5. 02694400	-3. 67958800
H	2. 99291400	5. 02367000	-2. 03422200
H	-0. 28525300	3. 80467100	-5. 24447700
C	0. 23361700	-3. 65840700	2. 40946600
C	-0. 13783700	-2. 69084400	3. 37327400
C	-0. 74082100	-4. 52641800	1. 85971300
C	0. 79897400	-1. 77732100	3. 95728200
C	-1. 51646400	-2. 59812900	3. 79788600
C	-2. 11742500	-4. 41626400	2. 28559700
C	0. 41171500	-0. 86344800	4. 90312000
H	1. 83116800	-1. 80553000	3. 62874200
C	-1. 87893300	-1. 63018100	4. 78731600
C	-2. 46658300	-3. 45877500	3. 24202700
C	-0. 94550000	-0. 78967200	5. 33035800
H	1. 14485700	-0. 17962200	5. 32084800
H	-2. 91940500	-1. 58186500	5. 10145000
H	-3. 50228200	-3. 38985000	3. 56980300
H	-1. 23364800	-0. 06085900	6. 08337900
C	6. 21981900	1. 98607600	-0. 08893500
H	7. 02503800	1. 48896500	0. 44514600
C	5. 42324900	1. 26744400	-0. 94116800
H	5. 61111400	0. 20963100	-1. 08261300
C	6. 00685500	3. 37981200	0. 10495800
H	6. 64706700	3. 93305900	0. 78698000
C	5. 00437500	4. 01645300	-0. 57519200
H	4. 82823300	5. 07961900	-0. 43677500
C	-1. 38403700	-6. 38240800	0. 40503600
H	-1. 11204400	-7. 14703600	-0. 31767700
C	-2. 74072100	-6. 26183800	0. 81974000
H	-3. 49065600	-6. 93366800	0. 41074600
C	-3. 09178400	-5. 30732400	1. 73572200
H	-4. 12205300	-5. 21205500	2. 07134500
C	-0. 42090000	-5. 54830300	0. 90911700

H	0.60836700	-5.65891700	0.58735400
N	0.63213700	-1.05243900	-1.76670100
S	-0.92071700	-1.08646400	-1.99991600
O	-1.33495800	-0.21619100	-3.10943500
O	-1.73434500	-0.98667300	-0.74917500
C	-1.31452800	-2.81013200	-2.60858100
F	-0.64333400	-3.06080200	-3.73805400
F	-2.62862100	-2.89549800	-2.85874600
F	-0.98718200	-3.72428600	-1.69419400
C	-5.12046900	1.15858700	-0.22778200
C	-5.08024500	2.58597900	-0.92432600
H	-5.59130300	3.27240500	-0.25075200
H	-5.70950300	2.51672300	-1.82355600
C	-3.78764100	3.19201900	-1.38275400
C	-4.09464400	1.15246400	0.93977800
H	-4.33099200	1.95211100	1.64165500
H	-4.16619500	0.20093200	1.47330400
N	-2.68714700	1.32612600	0.55641000
C	-1.81312100	2.13699000	1.20270600
N	-0.51517300	1.77727200	1.18093000
C	0.59105700	2.56870900	1.60565400
C	0.77601400	3.87796700	1.16050700
C	1.54449500	1.97192500	2.43677200
C	1.88472200	4.60570900	1.59150200
C	2.65768500	2.70543700	2.84361300
H	1.41355100	0.94218300	2.74368900
C	2.82945400	4.02963000	2.43878400
H	3.69322600	4.59616600	2.76499100
C	3.72400200	2.05729700	3.68751800
C	2.02508400	6.04166500	1.16550900
F	3.26129700	0.97326400	4.35223900
F	4.77238100	1.64714000	2.94282000
F	4.21306300	2.91791300	4.61074400
F	1.34677900	6.87871800	1.98239500
F	3.31416000	6.45162200	1.16815700
F	1.54067500	6.24538400	-0.08506400
S	-2.35750400	3.60984300	1.93950500
H	0.06827100	4.32792000	0.47831300
H	-0.24753700	0.79672600	0.96159700
H	-2.26828300	0.51611900	0.07071100
C	-3.35512200	4.43854700	-0.85547800
H	-2.95106000	4.00759900	0.26361100
C	-2.15437200	5.12744400	-1.50759000
H	-1.74369400	5.88386000	-0.83175400

H	-1.34759700	4.43918700	-1.77012000
H	-2.46034300	5.64257000	-2.42772100
C	-3.00733500	2.52545800	-2.47281700
H	-3.38701200	1.54454100	-2.74410500
H	-3.03833000	3.17319300	-3.36271800
H	-1.94631000	2.40873700	-2.23488700
C	-4.37461900	5.46520300	-0.32124700
H	-5.09269000	5.04585300	0.38499900
H	-3.83316800	6.25889500	0.20152900
H	-4.92609500	5.92251300	-1.15109300
C	-6.55461700	1.04870700	0.34005400
C	-7.64607800	1.07133400	-0.54580800
C	-6.84039200	0.95383600	1.70991000
C	-8.95979700	1.00775000	-0.08856500
H	-7.47267200	1.13151800	-1.61602600
C	-8.15798200	0.88361500	2.17344700
H	-6.04424400	0.92801800	2.44496700
C	-9.22431100	0.91282000	1.27925500
H	-9.77799000	1.02845000	-0.80368800
H	-8.34188800	0.80842700	3.24188100
H	-10.24785100	0.86123800	1.63991700
C	-4.86713200	0.00654000	-1.27563600
H	-3.78861700	-0.10534200	-1.41812100
H	-5.26200800	0.35560400	-2.23022400
C	-5.43675500	-1.37339600	-0.96788100
C	-6.34677700	-1.98213900	-1.76007200
C	-4.84296600	-2.04728000	0.25411600
H	-3.76870500	-1.84685800	0.31590000
H	-5.30819400	-1.69029200	1.18455500
H	-4.95120400	-3.13258000	0.23571900
C	-6.92589900	-1.41602200	-3.03974700
H	-6.85586400	-2.16296400	-3.84218600
H	-7.99639500	-1.19592500	-2.91753700
H	-6.43885300	-0.51007700	-3.40506200
C	-6.92237600	-3.35407200	-1.47198300
H	-6.55585000	-4.09352200	-2.19867700
H	-6.70417300	-3.72882400	-0.47165100
H	-8.01541600	-3.33085100	-1.58016400

TS-EF-7RS

l imaginary frequency

H = -5472.486434

G = -5472.700716

E(M06-2X-DCM) = -5473.463276

O	-0.43638500	-2.70167800	-1.08573100
O	-2.54075900	-1.46050700	-0.19243500
P	-0.90527600	-1.38220600	-0.23297300
O	-0.54231200	-0.09935400	-0.92192400
C	-1.55403600	-2.78698200	-5.11966900
C	-2.43842500	-3.19395300	-4.12583400
C	-2.02474200	-3.24766500	-2.78739100
C	0.17274300	-2.39514800	-3.42313800
C	-0.25292500	-2.43174900	-4.76371700
C	-3.17990900	-2.58578300	0.33348900
C	-3.30766600	-3.73193200	-0.45448800
C	-3.81294000	-4.90724600	0.12515300
C	-4.28037100	-4.91375200	1.43403600
C	-4.25738900	-3.72670400	2.16291100
C	-3.70758500	-2.54386100	1.64030200
H	0.45797700	-2.15144400	-5.53528300
H	-4.66011000	-3.70316600	3.17118100
C	-3.07807000	-3.95966400	-1.94813600
C	-4.36225300	-3.62978500	-2.78160700
H	-4.71425300	-2.62956200	-2.50361000
H	-5.17705000	-4.33550400	-2.59176400
H	-4.74790200	-6.30241200	-1.24507300
H	-3.36073500	-6.97619200	-0.39574200
C	-0.76163000	-2.77563200	-2.43951000
H	-1.86122200	-2.75789700	-6.16218900
H	-4.67247200	-5.82366300	1.88125900
C	-3.88403600	-3.62515900	-4.25136200
H	-4.47047000	-2.94844000	-4.88361500
H	-3.96482200	-4.62422500	-4.70215900
C	-3.75028800	-6.05931300	-0.85267900
C	-2.82919900	-5.50635300	-1.95867700
H	-1.78196900	-5.69377600	-1.69522100
H	-3.01066100	-5.95128200	-2.94192100
C	-3.80084900	-1.30655500	2.48118600
C	-3.08527100	-1.21868900	3.70027700
C	-4.73648600	-0.29918200	2.13356700
C	-2.10475500	-2.18586200	4.09013900
C	-3.33127100	-0.11222400	4.59892100
C	-4.95591200	0.81393500	3.03094900
C	-1.43422700	-2.08027700	5.27994200
H	-1.86632900	-2.99004900	3.40689500
C	-2.62107000	-0.04862100	5.83932900
C	-4.25632200	0.87231400	4.23984500
C	-1.70188500	-1.00544300	6.17435600

H	-0.67303300	-2.81180700	5.53314700
H	-2.82867400	0.78276100	6.50949600
H	-4.44646900	1.69777600	4.92386200
H	-1.16365000	-0.94326700	7.11636300
C	1.58344800	-2.00216500	-3.11656900
C	2.05759700	-0.72044400	-3.49572600
C	2.47450200	-2.94280000	-2.53969000
C	1.20939900	0.29286300	-4.05117900
C	3.45428300	-0.39112200	-3.31860700
C	3.85633800	-2.57849600	-2.32192500
C	1.70656900	1.50856400	-4.44579500
H	0.15105900	0.08712700	-4.15321400
C	3.93731400	0.88289000	-3.75883000
C	4.31139000	-1.32006100	-2.72360500
C	3.09280700	1.80787600	-4.31243800
H	1.03631700	2.25244800	-4.86914800
H	4.99722700	1.09535800	-3.64246800
H	5.35482900	-1.05424200	-2.56847900
H	3.47360200	2.76857300	-4.64912500
C	-6.43992600	0.62782600	0.64258200
H	-7.02587700	0.55969200	-0.26975500
C	-5.52480400	-0.34840700	0.93860700
H	-5.39644500	-1.18485000	0.26158400
C	-6.63616600	1.73231400	1.52025700
H	-7.36954200	2.49481600	1.27147200
C	-5.91220000	1.81824000	2.67924000
H	-6.06434800	2.64613500	3.36851800
C	2.96487100	-5.15149200	-1.61380300
H	2.63326600	-6.15139900	-1.34701100
C	4.31592400	-4.77469700	-1.37229400
H	5.00088700	-5.48475200	-0.91697800
C	4.74578500	-3.52453000	-1.72367700
H	5.77783800	-3.22461400	-1.55853100
C	2.08073200	-4.27107300	-2.17972800
H	1.06030400	-4.58493700	-2.36417400
C	-1.79980200	3.83822800	-0.46765600
C	-1.79146700	4.07707100	1.10669700
H	-1.64889400	5.14477200	1.26200200
H	-2.80124700	3.84413100	1.47135300
C	-0.85782300	3.31074100	2.00471300
C	-0.34748300	3.63253600	-0.97345600
H	0.24117500	4.52910200	-0.77921900
H	-0.36206400	3.47208800	-2.05408800
N	0.38440300	2.49900900	-0.39208700

C	1. 67183300	2. 55010700	-0. 00133800
N	2. 36758500	1. 40403900	0. 06285100
C	3. 73848900	1. 30271300	0. 47147600
C	4. 06792700	0. 70789300	1. 68933900
C	4. 73616800	1. 72624600	-0. 40361900
C	5. 41391300	0. 54646200	2. 02451500
C	6. 07656900	1. 54895300	-0. 06056600
H	4. 46157700	2. 16367100	-1. 35648300
C	6. 42314900	0. 96065300	1. 15510500
H	7. 46406500	0. 81644300	1. 41693100
C	7. 13105700	1. 92177500	-1. 06587800
C	5. 76603000	-0. 05231000	3. 36263200
F	7. 17738600	1. 02176500	-2. 08739800
F	8. 36480500	1. 96643400	-0. 52639100
F	6. 88349200	3. 12314900	-1. 63064000
F	5. 66508300	0. 86475300	4. 35375800
F	7. 03459000	-0. 51971700	3. 38576000
F	4. 94722000	-1. 07196300	3. 68336300
S	2. 37107300	4. 03904200	0. 57450600
H	3. 28470400	0. 35435200	2. 35104500
H	1. 91296200	0. 50621200	-0. 14009900
H	0. 02128500	1. 55651700	-0. 61903000
C	0. 17948000	3. 96166600	2. 69725800
H	1. 07973300	3. 97268700	1. 69163800
N	-0. 43200200	-1. 65968400	1. 28618900
S	1. 09129000	-1. 60953800	1. 71782900
O	1. 29030400	-0. 80191900	2. 93627400
O	2. 03945900	-1. 37004400	0. 60059300
C	1. 45199600	-3. 36508100	2. 24619300
F	0. 64673700	-3. 73175300	3. 25554700
F	2. 71996700	-3. 44878800	2. 65986300
F	1. 26646700	-4. 20247000	1. 22369000
C	0. 90633400	3. 21840300	3. 81886100
H	1. 09934600	2. 16826200	3. 59024300
H	1. 86780300	3. 69848100	4. 02495400
H	0. 31437600	3. 25267000	4. 74309500
C	-1. 16423300	1. 86517400	2. 25341900
H	-0. 28262900	1. 22671500	2. 34233900
H	-1. 68083300	1. 78984200	3. 22277900
H	-1. 82921900	1. 44056100	1. 50269500
C	0. 16934700	5. 48315600	2. 91809200
H	1. 15681100	5. 80221200	3. 26538100
H	-0. 05639500	6. 05721000	2. 01725800
H	-0. 55801400	5. 75392400	3. 69335600

C	-2.36664700	5.13890300	-1.08689200
C	-3.54662400	5.69924000	-0.56691200
C	-1.75734200	5.81217800	-2.15667700
C	-4.08945300	6.87417700	-1.08355500
H	-4.06022500	5.21223500	0.25641500
C	-2.29887900	6.98942200	-2.67998400
H	-0.84673100	5.43338700	-2.60593900
C	-3.46638400	7.52933400	-2.14671500
H	-5.00187400	7.27726300	-0.65165100
H	-1.79694900	7.48275100	-3.50817400
H	-3.88532300	8.44663800	-2.55102300
C	-2.74719100	2.63278400	-0.84953700
H	-3.63035200	2.71217700	-0.21250400
H	-2.25635000	1.69427100	-0.56931100
C	-3.17185700	2.52113800	-2.30991200
C	-4.41107100	2.82843100	-2.75123900
C	-2.11547000	1.96993400	-3.25544100
H	-2.54924900	1.33190200	-4.03057300
H	-1.55798500	2.76402600	-3.77495600
H	-1.39535600	1.35237300	-2.71289900
C	-4.80852700	2.73181200	-4.21040200
H	-5.50064800	1.89274700	-4.37617100
H	-5.34878000	3.63927600	-4.51205900
H	-3.96588600	2.61269700	-4.89294200
C	-5.56587500	3.29797000	-1.89604600
H	-6.47048100	2.72763000	-2.15022100
H	-5.40640600	3.19126000	-0.82260000
H	-5.79553800	4.35284800	-2.09843400

TS-EF-7RS-1

l imaginary frequency

H = -5472.483705

G = -5472.697765

E(M06-2X-DCM) = -5473.463114

O	-0.43117100	-2.75053300	-0.98231400
O	-2.54732400	-1.45120000	-0.20998100
P	-0.91120600	-1.39637100	-0.19262100
O	-0.50717300	-0.14336200	-0.91431600
C	-1.42336100	-2.99047000	-5.04343900
C	-2.34347200	-3.34615600	-4.06222700
C	-1.97273900	-3.34861600	-2.71003600
C	0.25441000	-2.54801900	-3.30992000
C	-0.12978400	-2.63599700	-4.66080500
C	-3.22257100	-2.54404400	0.33868200

C	-3.33794300	-3.72118300	-0.40361800
C	-3.87949200	-4.86415900	0.20677600
C	-4.39523200	-4.80747000	1.49624700
C	-4.38344400	-3.58983300	2.17315400
C	-3.79771000	-2.43779400	1.62115900
H	0.60860800	-2.39674200	-5.42017100
H	-4.82315000	-3.51731500	3.16344200
C	-3.06072400	-4.01465900	-1.87707400
C	-4.31371200	-3.70755400	-2.76512400
H	-4.66322600	-2.69303700	-2.54087500
H	-5.14210600	-4.39639900	-2.57244800
H	-4.78168100	-6.30858900	-1.13447300
H	-3.43256600	-6.95798800	-0.20846700
C	-0.71528700	-2.87598000	-2.34153900
H	-1.69677200	-3.00272300	-6.09565300
H	-4.81608600	-5.69200700	1.96758300
C	-3.78844400	-3.76961800	-4.21707200
H	-4.34738100	-3.11584500	-4.89660200
H	-3.86420400	-4.78634800	-4.62743000
C	-3.79577000	-6.05813400	-0.71792900
C	-2.83031200	-5.56285200	-1.81372300
H	-1.79507700	-5.75010400	-1.50642400
H	-2.98350100	-6.04735200	-2.78297500
C	-3.90174500	-1.16418800	2.40379600
C	-3.24160300	-1.04205900	3.65099300
C	-4.79328600	-0.14989000	1.97018800
C	-2.29441300	-2.00774900	4.11985400
C	-3.50918600	0.10108000	4.49583200
C	-5.03182100	1.00073400	2.81384700
C	-1.67769700	-1.86820000	5.33503100
H	-2.03536500	-2.83832400	3.47665300
C	-2.85755000	0.19863800	5.76587000
C	-4.39528100	1.08850800	4.05547800
C	-1.97068600	-0.75868900	6.17778600
H	-0.93953400	-2.59989700	5.64894100
H	-3.08207200	1.05710400	6.39516500
H	-4.60176500	1.94240600	4.69861800
H	-1.47626500	-0.67025200	7.14146600
C	1.66084400	-2.15821100	-2.98030100
C	2.16376800	-0.90482700	-3.41406500
C	2.52325200	-3.07927800	-2.33257400
C	1.34335000	0.09163200	-4.03736100
C	3.56181800	-0.58846600	-3.22582800
C	3.90517500	-2.72325700	-2.10122800

C	1. 86877500	1. 27550300	-4. 48733600
H	0. 28343200	-0. 10079700	-4. 14580400
C	4. 07532000	0. 65106000	-3. 72596800
C	4. 38999200	-1. 49634500	-2. 56145500
C	3. 25759500	1. 55803400	-4. 34565900
H	1. 21962000	2. 00781200	-4. 96116800
H	5. 13575200	0. 85356500	-3. 59891000
H	5. 43408600	-1. 23857200	-2. 39754700
H	3. 66129000	2. 49243100	-4. 72673300
C	-6. 38258200	0. 76665500	0. 35144400
H	-6. 91594900	0. 68135400	-0. 59130900
C	-5. 51551800	-0. 22300700	0. 73526900
H	-5. 37329200	-1. 08681600	0. 09654600
C	-6. 59823600	1. 90637400	1. 17774100
H	-7. 29339600	2. 67880600	0. 85989000
C	-5. 94051500	2. 01455300	2. 37385900
H	-6. 10890800	2. 87033100	3. 02421600
C	2. 95786000	-5. 24121200	-1. 27748000
H	2. 60478900	-6. 22051100	-0. 96563000
C	4. 30804100	-4. 87037400	-1. 02234400
H	4. 97075400	-5. 56382200	-0. 51185700
C	4. 76528400	-3. 64741800	-1. 43027200
H	5. 79745000	-3. 35320900	-1. 25582400
C	2. 10119500	-4. 38087300	-1. 91233000
H	1. 08116000	-4. 69063200	-2. 10529100
C	-1. 82633700	3. 89469200	-0. 52598300
C	-1. 70749900	4. 17739100	1. 02588400
H	-1. 43352100	5. 22435300	1. 13547700
H	-2. 71823200	4. 07728000	1. 44740500
C	-0. 82795500	3. 34394500	1. 91701300
C	-0. 42027000	3. 59476300	-1. 12647500
H	0. 20462400	4. 48677300	-1. 07639400
H	-0. 54216300	3. 32228500	-2. 17846800
N	0. 33170400	2. 49344400	-0. 50830100
C	1. 61796300	2. 55945200	-0. 12120900
N	2. 30886700	1. 41337900	-0. 00364500
C	3. 67221600	1. 32202500	0. 43393200
C	3. 97389800	0. 77631800	1. 68123000
C	4. 69017900	1. 70988200	-0. 43481500
C	5. 31176800	0. 62524400	2. 05254200
C	6. 02195600	1. 54482200	-0. 05470300
H	4. 43844300	2. 11063000	-1. 40959100
C	6. 34047300	1. 00385800	1. 19081100
H	7. 37507200	0. 87036900	1. 48186600

C	7. 10379800	1. 87094100	-1. 04708300
C	5. 62864800	0. 07534200	3. 42000700
F	7. 22803600	0. 88811900	-1. 98225800
F	8. 31099900	2. 00983700	-0. 46441600
F	6. 83875000	3. 00827600	-1. 72476100
F	5. 46432900	1. 01720400	4. 37894000
F	6. 90714100	-0. 35613000	3. 50515000
F	4. 82519200	-0. 95700800	3. 73954700
S	2. 31715500	4. 07014200	0. 39682900
H	3. 17679000	0. 45158400	2. 34054700
H	1. 84788900	0. 51397000	-0. 18003300
H	-0. 02767500	1. 53961500	-0. 68727000
C	0. 23117400	3. 93501600	2. 62677900
H	1. 10201500	3. 97380900	1. 57630200
N	-0. 49118300	-1. 62374700	1. 34946000
S	1. 01956100	-1. 54945600	1. 82459300
O	1. 18151900	-0. 68042100	3. 00630200
O	2. 00080100	-1. 36587500	0. 72710200
C	1. 35445700	-3. 27473400	2. 45768000
F	0. 50988900	-3. 58607900	3. 45315800
F	2. 60559400	-3. 33813100	2. 92296300
F	1. 20519300	-4. 16451900	1. 47402600
C	0. 95386600	3. 13331200	3. 70812700
H	1. 07858700	2. 07684800	3. 46337700
H	1. 94704000	3. 55720600	3. 88700100
H	0. 39864800	3. 18831200	4. 65408300
C	-1. 20707200	1. 91129900	2. 13709200
H	-0. 35876300	1. 23592500	2. 26092500
H	-1. 76783400	1. 85384200	3. 08287700
H	-1. 85590500	1. 51947200	1. 35557700
C	0. 28256800	5. 44664900	2. 90563400
H	1. 28773800	5. 71387000	3. 24577900
H	0. 06084000	6. 06866400	2. 03644200
H	-0. 41895100	5. 70903500	3. 70720400
C	-2. 34790800	5. 20526900	-1. 17258000
C	-3. 23605200	6. 05404900	-0. 48916100
C	-1. 98447800	5. 58488200	-2. 47596300
C	-3. 72665200	7. 22477200	-1. 06789400
H	-3. 56983300	5. 80537900	0. 51245500
C	-2. 47059400	6. 75623400	-3. 05912000
H	-1. 31798900	4. 96690700	-3. 06522700
C	-3. 34383700	7. 58657000	-2. 35848700
H	-4. 41159800	7. 85229700	-0. 50362800
H	-2. 16072200	7. 01586500	-4. 06797200

H	-3.72083400	8.49941200	-2.81129300
C	-2.82687500	2.69726000	-0.83460900
H	-3.52957900	2.63139100	0.00340100
H	-2.26685800	1.75895600	-0.82456000
C	-3.65854100	2.80309000	-2.10965800
C	-3.33670600	2.21512600	-3.28134600
C	-4.95735600	3.59102400	-1.97222300
H	-5.81571700	3.01477500	-2.33664800
H	-5.16019700	3.83665300	-0.92676400
H	-4.93773900	4.53708600	-2.52627400
C	-4.20054500	2.35182400	-4.51769500
H	-3.58035700	2.60412500	-5.38880000
H	-4.68974800	1.39612500	-4.75785700
H	-4.97673500	3.11418300	-4.43333800
C	-2.11927300	1.35767900	-3.52955500
H	-1.40460600	1.87759200	-4.18610400
H	-1.59254200	1.04092600	-2.62962800
H	-2.40809000	0.44289800	-4.06616200

TS-EF-7RS-2

l imaginary frequency

H = -5472.479376

G = -5472.693545

E(M06-2X-DCM) = -5473.456880

O	-0.76859000	-2.49758100	-1.22498000
O	-2.62500800	-1.42414500	0.25005300
P	-1.04252500	-1.28064500	-0.15806200
O	-0.87105800	0.08105800	-0.76611600
C	-2.84238300	-2.42540500	-4.85701300
C	-3.43843700	-2.92968200	-3.70526500
C	-2.70703700	-3.02935800	-2.51352200
C	-0.76860600	-2.03117300	-3.61107400
C	-1.50816700	-2.02043100	-4.80764000
C	-3.09385600	-2.60372700	0.83358300
C	-3.35619800	-3.71186400	0.02561300
C	-3.65888900	-4.94262800	0.63187400
C	-3.80502300	-5.04318400	2.01038400
C	-3.67398500	-3.89282600	2.78722000
C	-3.31724700	-2.65687800	2.22560700
H	-1.01968600	-1.66789500	-5.71127400
H	-3.83829300	-3.94101600	3.85986900
C	-3.48708500	-3.84650300	-1.49130900
C	-4.95061500	-3.55066800	-1.96515400
H	-5.26846500	-2.59023100	-1.54295300

H	-5.66083100	-4.31357800	-1.63123200
H	-4.82796100	-6.32188700	-0.56480300
H	-3.24603700	-6.94989400	-0.11485900
C	-1.41794200	-2.50665300	-2.45403600
H	-3.39725900	-2.36073000	-5.78970300
H	-4.03676000	-5.99682300	2.47792200
C	-4.85014000	-3.43755500	-3.50347400
H	-5.60348800	-2.76333100	-3.92718200
H	-4.99527500	-4.41361200	-3.98733400
C	-3.77826600	-6.03701600	-0.40575000
C	-3.17826700	-5.37268900	-1.66167300
H	-2.09091500	-5.51013600	-1.66825500
H	-3.57193200	-5.77593700	-2.59989400
C	-3.29772300	-1.44996700	3.11547200
C	-2.25811700	-1.25281500	4.05373600
C	-4.41353400	-0.57557500	3.09546000
C	-1.13770000	-2.13641600	4.15939100
C	-2.31350200	-0.12308300	4.95620400
C	-4.45252600	0.55556400	3.99504200
C	-0.14928700	-1.92461400	5.08294800
H	-1.06330600	-2.96749100	3.47128200
C	-1.26048600	0.06075800	5.90711600
C	-3.39761800	0.75734300	4.89073400
C	-0.21009900	-0.81425500	5.97227500
H	0.70309100	-2.59567900	5.11784000
H	-1.31920600	0.91157700	6.58255100
H	-3.43861800	1.60155600	5.57715200
H	0.58496200	-0.66344800	6.69770300
C	0.66172500	-1.59275700	-3.62108300
C	0.99625900	-0.27146000	-4.01495200
C	1.68937700	-2.52245800	-3.31802200
C	0.01270400	0.72184100	-4.33161300
C	2.38645800	0.11620700	-4.11495700
C	3.07234700	-2.10588500	-3.37520000
C	0.37126400	1.97085200	-4.77289100
H	-1.03564900	0.47260700	-4.21934600
C	2.71744000	1.43384900	-4.56326400
C	3.38374400	-0.80494300	-3.78104800
C	1.74290800	2.33492800	-4.89855300
H	-0.39983700	2.69205400	-5.03254400
H	3.76913500	1.69952600	-4.64252600
H	4.42875800	-0.50814500	-3.85070200
H	2.00954900	3.32593400	-5.25657900
C	-6.63228600	0.05444100	2.27915100

H	-7.48630900	-0.14028500	1.63573000
C	-5.55112700	-0.78809000	2.25088200
H	-5.55558100	-1.64646000	1.58854000
C	-6.65059100	1.18489700	3.14462200
H	-7.51372800	1.84533500	3.15136200
C	-5.58821700	1.42490900	3.97481800
H	-5.59658500	2.27484300	4.65382800
C	2.44461600	-4.75460100	-2.67093000
H	2.21378900	-5.78373600	-2.40963100
C	3.80091300	-4.32374100	-2.68551000
H	4.59130200	-5.02139500	-2.42289000
C	4.10371200	-3.03652600	-3.03515100
H	5.13422500	-2.69246600	-3.04963400
C	1.42906100	-3.88780400	-2.97696200
H	0.40482700	-4.24034300	-2.96468700
C	-1.28976700	4.01978600	-1.00575600
C	-1.65711100	3.89069300	0.54013600
H	-2.09496600	4.83574300	0.86636300
H	-2.44261400	3.13935600	0.62580100
C	-0.60118000	3.53603600	1.56588900
C	0.19879000	3.66204100	-1.27477400
H	0.84122400	4.49415800	-0.99523200
H	0.32821400	3.49280100	-2.34924400
N	0.72543700	2.47356200	-0.59167400
C	1.99128400	2.40663400	-0.12577400
N	2.56858800	1.20018100	-0.03026400
C	3.87831100	0.91133900	0.46587600
C	4.26440700	1.19963500	1.77443100
C	4.74995100	0.24756200	-0.39533600
C	5.54789500	0.85763700	2.19834000
C	6.02502900	-0.10631700	0.04528700
H	4.42260300	0.00314800	-1.39888600
C	6.43506200	0.20522700	1.34028600
H	7.42777000	-0.06381900	1.68155700
C	6.93589100	-0.87649100	-0.87367700
C	6.00222900	1.23731100	3.58349500
F	6.72637100	-2.20915200	-0.79127800
F	8.23768900	-0.66118000	-0.58972300
F	6.74209200	-0.53463200	-2.17261600
F	6.63460100	2.43502300	3.58390600
F	6.87206900	0.33634800	4.08898000
F	4.96830000	1.33834300	4.44463900
S	2.80738000	3.84259900	0.42211700
H	3.57012800	1.66829100	2.45828900

H	2.07767400	0.36139400	-0.36895400
H	0.24136300	1.57762000	-0.77036600
C	0.30773000	4.48588000	2.06154000
H	1.34877400	4.18124300	1.25982000
N	-0.22196800	-1.69271300	1.16827700
S	1.35508300	-1.83358400	1.20776800
O	1.93386000	-1.24206300	2.42097200
O	2.02152600	-1.51732200	-0.08540200
C	1.62224300	-3.67229600	1.40728800
F	1.09009400	-4.09379600	2.56671600
F	2.93287500	-3.93525300	1.42133100
F	1.05251100	-4.34757400	0.40563000
C	-1.53282900	5.46708000	-1.50099600
C	-0.69680600	6.08538900	-2.44711800
C	-2.64830400	6.20309600	-1.06134100
C	-0.94804500	7.37941100	-2.91080400
H	0.16997600	5.56886500	-2.84326300
C	-2.90197600	7.49466200	-1.52065400
H	-3.35518400	5.75508600	-0.37067100
C	-2.04897600	8.09532100	-2.44682600
H	-0.27261300	7.82402900	-3.63691600
H	-3.77434500	8.02933900	-1.15393500
H	-2.24268000	9.10305200	-2.80354700
C	-2.17300500	3.01320700	-1.85301900
H	-1.73249700	3.00948100	-2.85788700
H	-2.00340500	2.01151600	-1.45100600
C	-3.65909200	3.29498200	-2.01139500
C	-4.61778900	2.67644500	-1.28783700
C	-4.02821800	4.22608000	-3.16295300
H	-4.56393200	3.67974300	-3.95113600
H	-4.66883600	5.05998100	-2.85714900
H	-3.13909900	4.66626300	-3.62023700
C	-0.67979800	2.15115500	2.13652800
H	-1.06683900	1.43652800	1.40877500
H	0.27139800	1.77428000	2.51982700
H	-1.37863000	2.15818600	2.98855500
C	0.97200600	4.26780700	3.42543600
H	1.87080200	4.88702000	3.50760400
H	0.28618700	4.56879100	4.22766600
H	1.26338100	3.23169800	3.60651900
C	-6.09233700	2.93891300	-1.50893700
H	-6.56590800	2.07923700	-2.00593300
H	-6.60819900	3.05771500	-0.54665100
H	-6.29825400	3.82448300	-2.11331700

C	0.13111100	5.96879400	1.73151400
H	-0.20915200	6.14781900	0.71024900
H	-0.59464500	6.42630800	2.41705600
H	1.08118200	6.49712900	1.86426000
C	-4.37644500	1.62271000	-0.23390400
H	-3.35940600	1.23060200	-0.21072300
H	-4.63178300	1.99111100	0.76934900
H	-5.03979000	0.76587600	-0.40666600

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l imaginary frequency

H = -5472.482952

G = -5472.698314

E(M06-2X-DCM) = -5473.458643

O	-0.63773400	-2.43516600	-1.46682400
O	-2.71965400	-1.33393500	-0.35676400
P	-1.08110200	-1.27430200	-0.39473800
O	-0.68515000	0.10089500	-0.83728400
C	-1.85051300	-1.86608800	-5.43139500
C	-2.70395100	-2.44979600	-4.50027600
C	-2.25818000	-2.71072400	-3.19753200
C	-0.08881400	-1.73094900	-3.73147800
C	-0.54690800	-1.54834300	-5.04911100
C	-3.36626400	-2.52143500	-0.00081200
C	-3.48256400	-3.54981900	-0.93917000
C	-3.96460300	-4.80252200	-0.52529200
C	-4.42364900	-4.99762700	0.77204800
C	-4.43483200	-3.91563300	1.65075500
C	-3.91449800	-2.66195900	1.29103300
H	0.14086100	-1.13089100	-5.77865200
H	-4.84861900	-4.03166400	2.64834600
C	-3.27954500	-3.55917400	-2.45380700
C	-4.58782600	-3.13303200	-3.20344500
H	-4.95279500	-2.19622200	-2.76667300
H	-5.38447600	-3.87782900	-3.11046200
H	-4.89543000	-6.01525500	-2.06183700
H	-3.47756300	-6.76720600	-1.33843300
C	-0.99364100	-2.28293600	-2.80413800
H	-2.18304800	-1.67122800	-6.44797300
H	-4.79230400	-5.96857900	1.09305900
C	-4.14344100	-2.88850900	-4.66359600
H	-4.75778300	-2.13577500	-5.17103700
H	-4.21366400	-3.80715300	-5.26291900
C	-3.89563700	-5.80515900	-1.65620100

C	-3.00816100	-5.08300800	-2.69058200
H	-1.95246800	-5.28721400	-2.47837400
H	-3.20608100	-5.38611900	-3.72351000
C	-4.09593400	-1.52823100	2.25734300
C	-3.31848200	-1.43920300	3.43530100
C	-5.18063100	-0.63752400	2.05232800
C	-2.24425700	-2.34094900	3.71887800
C	-3.60918400	-0.40948700	4.40972400
C	-5.47092700	0.37647700	3.04162900
C	-1.50763200	-2.23140100	4.86836800
H	-1.99758500	-3.10084400	2.98999000
C	-2.81558200	-0.33073000	5.59798100
C	-4.67032300	0.47149400	4.18382200
C	-1.79553500	-1.21521800	5.82338200
H	-0.68063300	-2.91286700	5.04094400
H	-3.05040500	0.44535200	6.32334700
H	-4.89729700	1.23214200	4.92888400
H	-1.19959000	-1.14572100	6.72959800
C	1.32787200	-1.38732200	-3.39580800
C	1.78766700	-0.05446000	-3.54486600
C	2.23702900	-2.41202400	-3.02864200
C	0.91955600	1.03620700	-3.87931700
C	3.18972500	0.24584700	-3.35518700
C	3.62647400	-2.08664700	-2.79842800
C	1.40515600	2.30555600	-4.06950200
H	-0.14242200	0.84446600	-3.97748000
C	3.65563800	1.58349600	-3.56280800
C	4.06822600	-0.77334300	-2.97829100
C	2.79419500	2.58660900	-3.91889200
H	0.72387500	3.10704100	-4.34563800
H	4.71898200	1.77896000	-3.44090600
H	5.11845800	-0.53751900	-2.82027900
H	3.16326700	3.59508800	-4.08586000
C	-7.12784100	0.11663900	0.77645200
H	-7.77880400	0.01828700	-0.08832200
C	-6.05379400	-0.72371100	0.91951900
H	-5.86370500	-1.48356200	0.17015000
C	-7.40608000	1.11499200	1.75335100
H	-8.26449500	1.76942600	1.62670600
C	-6.59463200	1.24038300	2.84892100
H	-6.79890100	1.99351100	3.60681100
C	2.75514800	-4.74872200	-2.53242200
H	2.43106300	-5.78148600	-2.43642700
C	4.11557100	-4.41590400	-2.27858500

H	4.81514700	-5.19351700	-1.98440800
C	4.53568900	-3.12141200	-2.41523200
H	5.57395800	-2.85194300	-2.23718100
C	1.85300400	-3.78488800	-2.89835500
H	0.82555600	-4.06429000	-3.09778300
C	-1.11568100	4.08497900	-0.26257400
C	-1.27238300	4.14379500	1.31924400
H	-1.08048100	5.17226900	1.61784900
H	-2.32460000	3.94806700	1.55248900
C	-0.47923400	3.21914000	2.20713500
C	0.33511100	3.69941500	-0.65370700
H	1.02875900	4.48029100	-0.34365200
H	0.39029600	3.61307700	-1.74388000
N	0.84563100	2.42900500	-0.12024200
C	2.10562800	2.27568300	0.33555800
N	2.65181200	1.05176400	0.31754500
C	3.98860700	0.74387300	0.72396500
C	4.21433300	-0.09581600	1.81437600
C	5.05356400	1.20023600	-0.05051500
C	5.52321800	-0.47412000	2.12096700
C	6.35510800	0.81360800	0.26611300
H	4.85655700	1.82612400	-0.91329600
C	6.59826900	-0.02545600	1.35333200
H	7.60726700	-0.34156000	1.58664000
C	7.47654300	1.30078900	-0.61033200
C	5.75803900	-1.36359300	3.31559300
F	7.19335500	1.09430300	-1.92501400
F	8.64193600	0.67733100	-0.34840900
F	7.68567100	2.62784100	-0.47037600
F	5.67573200	-0.66669900	4.47279500
F	6.98202000	-1.93644400	3.28429400
F	4.84449900	-2.35203000	3.38459000
S	2.94092500	3.60526100	1.09015600
H	3.37622800	-0.46465800	2.39611900
H	2.10276600	0.22961500	0.03100900
H	0.36654000	1.57615700	-0.45462500
C	0.56869800	3.70970100	3.01067700
H	1.54157200	3.65520000	2.09048500
N	-0.60474700	-1.83918200	1.04401400
S	0.91690300	-1.90896300	1.45793200
O	1.18698200	-1.23664400	2.74430600
O	1.87249200	-1.61962400	0.35498800
C	1.18820600	-3.72220600	1.80963100
F	0.36333500	-4.14407100	2.78146500

F	2. 44996800	-3. 90631300	2. 21099700
F	0. 96547900	-4. 44686400	0. 71180900
C	1. 11981000	2. 83324100	4. 13815800
H	1. 25273400	1. 78868300	3. 84936100
H	2. 09229100	3. 21342300	4. 46475100
H	0. 44541000	2. 85658000	5. 00405500
C	-0. 93941200	1. 79611400	2. 31823000
H	-0. 13884100	1. 07958300	2. 51324000
H	-1. 62369300	1. 72560300	3. 17959000
H	-1. 48831800	1. 46264400	1. 43889000
C	0. 70243200	5. 21015400	3. 31799100
H	1. 68308000	5. 39978700	3. 76478400
H	0. 62280800	5. 84620100	2. 43401500
H	-0. 05832300	5. 52579100	4. 04264100
C	-1. 40161600	5. 50744500	-0. 79849900
C	-2. 49703000	6. 23748600	-0. 30257700
C	-0. 62793400	6. 11822300	-1. 79876600
C	-2. 80219800	7. 51219800	-0. 77655500
H	-3. 12994800	5. 80721900	0. 46582500
C	-0. 92903700	7. 39685800	-2. 27586800
H	0. 22956300	5. 61189600	-2. 22653300
C	-2. 01782700	8. 10186800	-1. 76915800
H	-3. 65643300	8. 04462200	-0. 36639700
H	-0. 30221000	7. 83792600	-3. 04642400
H	-2. 25152100	9. 09664100	-2. 13845100
C	-2. 09387200	3. 06694800	-0. 96987900
H	-1. 89327400	2. 06177100	-0. 58731500
H	-1. 77229500	3. 03615200	-2. 01459700
C	-3. 59157500	3. 31581500	-0. 90249800
C	-4. 29179800	3. 88378300	-1. 90911100
C	-4. 28517700	2. 82009700	0. 35795000
H	-5. 20586400	2. 27364500	0. 13970700
H	-3. 64885000	2. 12783000	0. 91500700
H	-4. 55979200	3. 63495500	1. 04440400
C	-5. 78634500	4. 11179600	-1. 84155400
H	-6. 01208900	5. 18151000	-1. 95894500
H	-6. 29520800	3. 59934100	-2. 67047300
H	-6. 24414500	3. 77866500	-0. 90908400
C	-3. 70638500	4. 38690100	-3. 20857100
H	-3. 81415800	5. 47813900	-3. 27856500
H	-2. 64856300	4. 15942000	-3. 34366500
H	-4. 25430700	3. 96236500	-4. 06143800

l imaginary frequency

H = -5472.482952

G = -5472.698316

E(M06-2X-DCM) = -5473.458642

O	-0.63778000	-2.43513600	-1.46684400
O	-2.71969900	-1.33392100	-0.35676900
P	-1.08114600	-1.27430200	-0.39472400
O	-0.68518700	0.10091100	-0.83721200
C	-1.85056900	-1.86600500	-5.43140400
C	-2.70400600	-2.44972400	-4.50029100
C	-2.25823600	-2.71066900	-3.19755000
C	-0.08886600	-1.73089600	-3.73148800
C	-0.54696100	-1.54827100	-5.04911800
C	-3.36632500	-2.52141500	-0.00083300
C	-3.48262800	-3.54978900	-0.93920000
C	-3.96467900	-4.80249100	-0.52533800
C	-4.42373800	-4.99760300	0.77199600
C	-4.43492100	-3.91561600	1.65071200
C	-3.91457200	-2.66194300	1.29100600
H	0.14080900	-1.13081400	-5.77865600
H	-4.84871900	-4.03165100	2.64829900
C	-3.27960200	-3.55912700	-2.45383600
C	-4.58788300	-3.13297400	-3.20347000
H	-4.95285200	-2.19616900	-2.76668700
H	-5.38453300	-3.87777100	-3.11049700
H	-4.89550000	-6.01520800	-2.06190000
H	-3.47763900	-6.76716900	-1.33849600
C	-0.99369500	-2.28288800	-2.80415200
H	-2.18310500	-1.67113200	-6.44797900
H	-4.79240400	-5.96855400	1.09299700
C	-4.14349700	-2.88843300	-4.66361800
H	-4.75783700	-2.13569100	-5.17104900
H	-4.21372000	-3.80706900	-5.26295300
C	-3.89570900	-5.80511800	-1.65625600
C	-3.00822500	-5.08296000	-2.69062600
H	-1.95253300	-5.28717300	-2.47841600
H	-3.20614100	-5.38606000	-3.72355800
C	-4.09600400	-1.52821700	2.25732000
C	-3.31856200	-1.43920500	3.43528600
C	-5.18068100	-0.63748800	2.05229300
C	-2.24435400	-2.34096800	3.71887200
C	-3.60925700	-0.40948400	4.40970700
C	-5.47096800	0.37651800	3.04159100
C	-1.50773900	-2.23143300	4.86836900

H	-1.99768600	-3.10086500	2.98998500
C	-2.81566600	-0.33074300	5.59797200
C	-4.67037700	0.47151700	4.18379400
C	-1.79563500	-1.21524700	5.82338300
H	-0.68075300	-2.91291200	5.04095300
H	-3.05048300	0.44534300	6.32333700
H	-4.89734400	1.23216800	4.92885400
H	-1.19969900	-1.14576200	6.72960500
C	1.32782400	-1.38729000	-3.39581800
C	1.78763600	-0.05443100	-3.54486000
C	2.23697000	-2.41200800	-3.02866900
C	0.91953700	1.03625000	-3.87929500
C	3.18969800	0.24585500	-3.35518300
C	3.62642000	-2.08665200	-2.79845800
C	1.40515200	2.30559600	-4.06946600
H	-0.14244300	0.84452300	-3.97746000
C	3.65562600	1.58350100	-3.56278700
C	4.06818800	-0.77335100	-2.97830500
C	2.79419500	2.58663000	-3.91885600
H	0.72388000	3.10709200	-4.34559100
H	4.71897400	1.77895100	-3.44088700
H	5.11842400	-0.53754200	-2.82029500
H	3.16327900	3.59510600	-4.08581200
C	-7.12785600	0.11672200	0.77639000
H	-7.77880800	0.01838600	-0.08839400
C	-6.05383000	-0.72365400	0.91947100
H	-5.86374900	-1.48350800	0.17010400
C	-7.40608600	1.11507900	1.75328700
H	-8.26448500	1.76953300	1.62663000
C	-6.59465200	1.24044800	2.84887000
H	-6.79891500	1.99357900	3.60675800
C	2.75506300	-4.74872000	-2.53248600
H	2.43096600	-5.78148100	-2.43650500
C	4.11549100	-4.41592100	-2.27865000
H	4.81505900	-5.19354800	-1.98448600
C	4.53562400	-3.12143300	-2.41528000
H	5.57389700	-2.85197900	-2.23722900
C	1.85293000	-3.78486900	-2.89840200
H	0.82547700	-4.06425600	-3.09783000
C	-1.11558500	4.08501400	-0.26253000
C	-1.27226500	4.14392000	1.31929000
H	-1.08036000	5.17241000	1.61783500
H	-2.32448000	3.94820500	1.55255900
C	-0.47910600	3.21931200	2.20721900

C	0.33519500	3.69940700	-0.65366600
H	1.02886200	4.48027100	-0.34362000
H	0.39037400	3.61306400	-1.74383800
N	0.84569400	2.42898900	-0.12020300
C	2.10569500	2.27564400	0.33557800
N	2.65184600	1.05170900	0.31757100
C	3.98863700	0.74377900	0.72397000
C	4.21434800	-0.09594500	1.81435800
C	5.05360100	1.20013400	-0.05050400
C	5.52322500	-0.47429500	2.12092800
C	6.35513600	0.81346400	0.26610500
H	4.85660600	1.82605100	-0.91326800
C	6.59828300	-0.02563800	1.35329900
H	7.60727300	-0.34177800	1.58658800
C	7.47657600	1.30063600	-0.61033800
C	5.75802900	-1.36379500	3.31553800
F	7.19338900	1.09415500	-1.92502000
F	8.64196500	0.67716900	-0.34841500
F	7.68571400	2.62768600	-0.47037900
F	5.67585500	-0.66689900	4.47274900
F	6.98195400	-1.93676300	3.28416800
F	4.84439800	-2.35214400	3.38458200
S	2.94104700	3.60521400	1.09012800
H	3.37623700	-0.46477800	2.39609700
H	2.10277500	0.22957500	0.03104200
H	0.36657600	1.57615500	-0.45458000
C	0.56887500	3.70990800	3.01067500
H	1.54169900	3.65528800	2.09046900
N	-0.60480300	-1.83924500	1.04400800
S	0.91684300	-1.90898100	1.45794800
O	1.18690800	-1.23661500	2.74430000
O	1.87243800	-1.61966700	0.35500400
C	1.18816400	-3.72220800	1.80971300
F	0.36327400	-4.14405800	2.78153700
F	2.44991800	-3.90627900	2.21112000
F	0.96548200	-4.44690500	0.71190800
C	1.12000400	2.83354200	4.13822300
H	1.25280500	1.78893400	3.84955500
H	2.09254800	3.21367800	4.46468200
H	0.44567800	2.85706300	5.00417400
C	-0.93931000	1.79630400	2.31842100
H	-0.13875700	1.07977300	2.51350200
H	-1.62361200	1.72587700	3.17977000
H	-1.48820400	1.46277700	1.43909400

C	0.70266200	5.21038300	3.31786000
H	1.68335000	5.40003200	3.76455900
H	0.62297900	5.84636300	2.43384100
H	-0.05802900	5.52608900	4.04254800
C	-1.40150300	5.50746100	-0.79851500
C	-2.49692900	6.23751800	-0.30264200
C	-0.62779400	6.11820900	-1.79878000
C	-2.80208500	7.51221600	-0.77666600
H	-3.12986400	5.80727600	0.46576000
C	-0.92888700	7.39683000	-2.27592900
H	0.22971500	5.61187200	-2.22650800
C	-2.01769000	8.10185500	-1.76926800
H	-3.65632900	8.04465400	-0.36654400
H	-0.30204000	7.83787500	-3.04648200
H	-2.25137500	9.09661600	-2.13859800
C	-2.09379900	3.06696100	-0.96977100
H	-1.89320700	2.06179900	-0.58716400
H	-1.77224100	3.03611200	-2.01449200
C	-3.59150100	3.31583900	-0.90237600
C	-4.29173900	3.88375500	-1.90900900
C	-4.28507700	2.82019000	0.35811500
H	-5.20569000	2.27359700	0.13991100
H	-3.64868600	2.12806800	0.91527700
H	-4.55981500	3.63510100	1.04445600
C	-5.78628000	4.11179000	-1.84143900
H	-6.01196600	5.18160200	-1.95808500
H	-6.29507600	3.59995800	-2.67077900
H	-6.24419200	3.77801300	-0.90925600
C	-3.70633300	4.38685000	-3.20848100
H	-3.81436100	5.47805500	-3.27861200
H	-2.64844400	4.15961400	-3.34345300
H	-4.25408000	3.96208500	-4.06134600

TS-EF-7RR

l imaginary frequency

H = -5472.485856

G = -5472.701308

E(M06-2X-DCM) = -5473.463093

O	-1.07280800	-2.18585400	-1.61054700
O	-2.92277900	-0.75883100	-0.47118400
P	-1.30344600	-1.02519000	-0.46947200
O	-0.61557500	0.25594900	-0.82398300
C	-2.07632600	-1.15430900	-5.54109500
C	-3.04088100	-1.63107900	-4.65850500

C	-2.67834300	-2.04607400	-3.36973000
C	-0.35775700	-1.44025600	-3.81561900
C	-0.74627500	-1.09718500	-5.12351400
C	-3.79819100	-1.81047700	-0.18626100
C	-4.08610900	-2.75325600	-1.17633000
C	-4.80646200	-3.90926400	-0.83418700
C	-5.32775200	-4.07223600	0.44393200
C	-5.15711300	-3.04834400	1.37442800
C	-4.39839800	-1.90207500	1.08713300
H	0.02079800	-0.76256300	-5.81577100
H	-5.61183200	-3.12849700	2.35764300
C	-3.85392800	-2.72931600	-2.68646300
C	-5.04558800	-2.03243600	-3.42851000
H	-5.24470800	-1.06941200	-2.94383100
H	-5.96631300	-2.62277600	-3.38769100
H	-5.90780100	-4.85560500	-2.44426400
H	-4.67227000	-5.89066200	-1.73658900
C	-1.36554500	-1.88229900	-2.93619400
H	-2.34570400	-0.84257900	-6.54722500
H	-5.88133100	-4.96896800	0.71064300
C	-4.53116200	-1.79558000	-4.86639000
H	-4.99059200	-0.92093900	-5.34137300
H	-4.74870700	-2.65530200	-5.51567200
C	-4.89682400	-4.85402600	-2.01272300
C	-3.86502700	-4.26370000	-2.99628500
H	-2.87128800	-4.67146200	-2.77878700
H	-4.09130800	-4.47595700	-4.04602000
C	-4.38672900	-0.79994300	2.10568800
C	-3.64318400	-0.91819800	3.30294500
C	-5.27270800	0.29272500	1.92422400
C	-2.77315300	-2.02422500	3.56292800
C	-3.75989800	0.10187100	4.32279500
C	-5.38423800	1.30248100	2.95278300
C	-2.06767700	-2.11503300	4.73336300
H	-2.65288200	-2.78130700	2.79999300
C	-3.00753200	-0.03301700	5.53247200
C	-4.61705800	1.18652700	4.11591500
C	-2.18621800	-1.10942700	5.73464000
H	-1.39323200	-2.95125800	4.88793000
H	-3.11245600	0.73814100	6.29276700
H	-4.71474500	1.94246200	4.89340300
H	-1.62019800	-1.20171400	6.65789000
C	1.08783600	-1.36431900	-3.43896000
C	1.76599700	-0.12024300	-3.48303700

C	1. 80279200	-2. 54939100	-3. 13064100
C	1. 10174400	1. 12144300	-3. 75213100
C	3. 19117500	-0. 07208300	-3. 24286400
C	3. 21916700	-2. 47783900	-2. 85182300
C	1. 79297500	2. 30446900	-3. 82578500
H	0. 02791300	1. 11513000	-3. 89726900
C	3. 87718900	1. 18119400	-3. 33699100
C	3. 87702100	-1. 24732800	-2. 92507900
C	3. 20351700	2. 33804500	-3. 62518000
H	1. 26128200	3. 22718000	-4. 04539700
H	4. 95370200	1. 18688700	-3. 18035500
H	4. 94547100	-1. 20101100	-2. 72631500
H	3. 73845600	3. 28101500	-3. 70337700
C	-7. 01629200	1. 45445200	0. 66072200
H	-7. 66350000	1. 51241700	-0. 21076500
C	-6. 12495000	0. 41967700	0. 77968400
H	-6. 07163300	-0. 33483200	0. 00322300
C	-7. 11162900	2. 45267300	1. 67159700
H	-7. 82722800	3. 26377500	1. 56361400
C	-6. 31119200	2. 37772900	2. 77988100
H	-6. 38105600	3. 12654400	3. 56591500
C	1. 91042900	-4. 96812600	-2. 79638300
H	1. 41673200	-5. 93606600	-2. 78131000
C	3. 29912400	-4. 88634400	-2. 49500000
H	3. 85083000	-5. 78865200	-2. 24582800
C	3. 93216200	-3. 67428900	-2. 52891200
H	4. 99487100	-3. 59568800	-2. 31266700
C	1. 19194800	-3. 84379300	-3. 10692400
H	0. 13841600	-3. 93202600	-3. 34351200
C	-0. 49063700	4. 45158500	0. 26472700
C	-0. 43197600	4. 45960300	1. 83771900
H	0. 30978800	5. 20707400	2. 11987500
H	-1. 39263300	4. 83834300	2. 21160600
C	-0. 15389200	3. 17762700	2. 57915500
C	0. 77187700	3. 75592400	-0. 30104800
H	1. 63985300	4. 34426100	-0. 00822000
H	0. 73170400	3. 76517600	-1. 39358900
N	1. 05064400	2. 37254500	0. 11894200
C	2. 24394500	1. 97084900	0. 59602300
N	2. 59238500	0. 68197200	0. 47027000
C	3. 85475900	0. 13678100	0. 87308200
C	3. 92727500	-0. 78672700	1. 91531600
C	4. 99291200	0. 46752700	0. 14067100
C	5. 15642100	-1. 37787700	2. 21474600

C	6.21368400	-0.13209700	0.44869100
H	4.91204100	1.16774100	-0.68289300
C	6.30315200	-1.05829300	1.48720800
H	7.24719700	-1.53713200	1.71485700
C	7.41246300	0.22381400	-0.38694600
C	5.22708400	-2.35734700	3.35874500
F	7.14958600	0.06438800	-1.71330500
F	8.48645600	-0.53656600	-0.09866500
F	7.77286600	1.51565700	-0.22560200
F	5.21308400	-1.72146200	4.55361700
F	6.35658600	-3.09920200	3.31829900
F	4.17960400	-3.20506300	3.35123400
S	3.24322500	3.06170000	1.52447500
H	3.03171200	-1.05502900	2.46494800
H	1.93898300	-0.00321600	0.07197500
H	0.44680300	1.63433500	-0.28059500
C	0.90102500	3.10868100	3.50579300
H	1.88197700	3.10553600	2.55755600
N	-0.99952300	-1.75954600	0.93752400
S	0.47128700	-2.09963700	1.40356500
O	0.78399000	-1.54323700	2.73541700
O	1.51003300	-1.92138600	0.35683000
C	0.41449200	-3.94569900	1.67395800
F	-0.51649100	-4.26164500	2.58875100
F	1.60585500	-4.36046500	2.11687600
F	0.12704600	-4.57482400	0.53289900
C	-1.82142300	3.90791000	-0.28354600
C	-1.88612200	3.00929900	-1.35570100
C	-3.03985200	4.38415600	0.23441000
C	-3.11199800	2.59540800	-1.88358400
H	-0.98722100	2.59286000	-1.79069700
C	-4.26358600	3.98059100	-0.29207700
H	-3.04565600	5.09333900	1.05827400
C	-4.30567400	3.08093700	-1.35881400
H	-3.12076600	1.87496900	-2.69629900
H	-5.18507500	4.35612800	0.14232300
H	-5.25968300	2.75160400	-1.75907400
C	-0.36162200	5.97891700	-0.14673600
H	-1.21000000	6.50079300	0.31367400
H	0.53510800	6.36596300	0.34630400
C	-0.33091200	6.32411200	-1.62969700
C	0.81387100	6.59452300	-2.29751000
C	0.84341400	6.92814600	-3.77522500
H	1.08678600	7.98913900	-3.93335300

H	1.63629700	6.35596400	-4.27577900
H	-0.09153800	6.71530800	-4.29534700
C	1.10430900	1.83286900	4.32256200
H	1.07168500	0.91971300	3.72368300
H	2.07561000	1.86601400	4.82566400
H	0.33243300	1.74142800	5.09765500
C	-1.68993700	6.41759800	-2.30850600
H	-1.98348600	5.47878700	-2.79349000
H	-2.47153500	6.63943200	-1.57588100
H	-1.71932200	7.20719900	-3.06440500
C	-1.07072200	2.01328700	2.35885700
H	-0.58715900	1.04457100	2.49647000
H	-1.86181900	2.06710600	3.12493100
H	-1.56293800	2.03032600	1.38778200
C	1.41493500	4.34648800	4.25717600
H	2.45604300	4.18862900	4.55659000
H	1.37247100	5.27563400	3.68738500
H	0.82514400	4.48230300	5.17238300
C	2.20201500	6.61535900	-1.69422700
H	2.22324600	6.60767100	-0.60282600
H	2.79628100	5.75729700	-2.03951600
H	2.73942800	7.51365300	-2.02691000

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1 imaginary frequency

H = -5472.484135

G = -5472.698775

E(M06-2X-DCM) = -5473.462559

O	-0.83060400	-2.21409000	-1.60656200
O	-2.79223700	-0.99655400	-0.40828300
P	-1.15430000	-1.09185800	-0.44937800
O	-0.61065000	0.25614900	-0.80287400
C	-2.00091200	-1.24686800	-5.50638500
C	-2.89916500	-1.82074900	-4.61161500
C	-2.47335300	-2.21312200	-3.33539600
C	-0.22886100	-1.38889100	-3.81716100
C	-0.67345200	-1.07140300	-5.11370600
C	-3.54897500	-2.13670800	-0.12594200
C	-3.76002500	-3.08841700	-1.12735700
C	-4.35327800	-4.31672300	-0.79291700
C	-4.82871800	-4.55315700	0.49150800
C	-4.74475800	-3.53203600	1.43654300
C	-4.11351500	-2.30944000	1.15564200
H	0.04557500	-0.66199400	-5.81726900

H	-5.17017900	-3.67324400	2.42600300
C	-3.56278600	-3.01683300	-2.64113500
C	-4.83102500	-2.42825600	-3.34890800
H	-5.11137100	-1.49560900	-2.84543900
H	-5.68973200	-3.10517600	-3.29985700
H	-5.39014200	-5.34086100	-2.39771400
H	-4.04297600	-6.25970400	-1.73465500
C	-1.17436800	-1.92945600	-2.92372000
H	-2.31777200	-0.95194800	-6.50373900
H	-5.28284900	-5.50584200	0.75200400
C	-4.37132200	-2.12331300	-4.79276400
H	-4.92139100	-1.28950800	-5.24435900
H	-4.52035100	-2.99033900	-5.45159000
C	-4.37504600	-5.24604700	-1.98672100
C	-3.42883600	-4.53957500	-2.97918100
H	-2.39506400	-4.84995700	-2.78921200
H	-3.65539300	-4.75566900	-4.02804400
C	-4.20447400	-1.22758500	2.19229600
C	-3.42022000	-1.27067600	3.36819600
C	-5.22260700	-0.24987900	2.05298100
C	-2.42006900	-2.26982300	3.58980100
C	-3.62957800	-0.28410500	4.40615100
C	-5.42880000	0.72388100	3.10143200
C	-1.67629500	-2.28958500	4.73972000
H	-2.23472200	-3.00034400	2.81423400
C	-2.83187400	-0.34153600	5.59283000
C	-4.61848400	0.68974900	4.24030100
C	-1.88344000	-1.31505700	5.75725000
H	-0.90510000	-3.04292500	4.86498900
H	-3.00613600	0.40282700	6.36694900
H	-4.78505200	1.41826100	5.03208500
H	-1.28472900	-1.34984400	6.66370300
C	1.21103400	-1.18638200	-3.46647000
C	1.77549100	0.11312500	-3.51452700
C	2.03421300	-2.30477000	-3.17923200
C	0.99954100	1.29150300	-3.76838600
C	3.19469800	0.28689500	-3.29839600
C	3.44319200	-2.10871000	-2.92362400
C	1.58295600	2.53060400	-3.85269800
H	-0.07192100	1.19010600	-3.89399800
C	3.76539500	1.59623700	-3.39914500
C	3.98762000	-0.82408000	-2.99927500
C	2.98794700	2.68928500	-3.67455100
H	0.96859200	3.40173000	-4.06825900

H	4. 83958700	1. 69689900	-3. 25978500
H	5. 05115800	-0. 68383400	-2. 81903500
H	3. 43553400	3. 67603900	-3. 75838900
C	-7. 13397800	0. 70170300	0. 85729900
H	-7. 80752500	0. 69123900	0. 00416600
C	-6. 11593900	-0. 21352400	0. 93333300
H	-5. 98957500	-0. 94302900	0. 14157100
C	-7. 32584900	1. 66396000	1. 88960400
H	-8. 14133600	2. 37891900	1. 81646700
C	-6. 48908000	1. 67539300	2. 97371800
H	-6. 63023200	2. 39745100	3. 77509400
C	2. 36336400	-4. 70632700	-2. 86595000
H	1. 95845000	-5. 71462800	-2. 85053900
C	3. 74412600	-4. 50258500	-2. 58683900
H	4. 37845800	-5. 35346500	-2. 35392400
C	4. 26563400	-3. 23856400	-2. 62179100
H	5. 32068000	-3. 06659100	-2. 42282800
C	1. 54209300	-3. 64878600	-3. 15558500
H	0. 49687600	-3. 82960700	-3. 37570800
C	-0. 84542400	4. 34766300	0. 35419900
C	-0. 75129800	4. 34034800	1. 92358900
H	-0. 07917800	5. 15522300	2. 19283900
H	-1. 72957400	4. 62354500	2. 33395700
C	-0. 31961300	3. 08765500	2. 64380700
C	0. 49294200	3. 83195500	-0. 22601600
H	1. 28818200	4. 50477700	0. 09345100
H	0. 46180900	3. 86442600	-1. 31727800
N	0. 91558000	2. 47326800	0. 14987700
C	2. 15071900	2. 17865900	0. 59655900
N	2. 62121100	0. 93420500	0. 42978800
C	3. 93848000	0. 50402500	0. 79323600
C	4. 12184100	-0. 43793700	1. 80519600
C	5. 02336400	0. 96345700	0. 04962000
C	5. 40788000	-0. 91718600	2. 06207200
C	6. 30212500	0. 47410300	0. 31470500
H	4. 85847900	1. 67621300	-0. 75040700
C	6. 50245900	-0. 46908200	1. 32174500
H	7. 49258200	-0. 86219100	1. 51544100
C	7. 43986600	0. 96070900	-0. 54009200
C	5. 59938200	-1. 91525700	3. 17580900
F	7. 17590400	0. 76687000	-1. 86176400
F	8. 59772600	0. 32864200	-0. 26761200
F	7. 65235200	2. 28587200	-0. 38753000
F	5. 58491800	-1. 31128100	4. 38710200

F	6.78053800	-2.56491800	3.07201500
F	4.62132200	-2.84206300	3.18550400
S	3.05523700	3.33898800	1.53838800
H	3.26841100	-0.80545800	2.36426200
H	2.02744500	0.19636500	0.03176300
H	0.37281000	1.69404500	-0.26163000
C	0.75074900	3.12908900	3.55419500
H	1.71468400	3.23524200	2.58944600
N	-0.74218500	-1.80565500	0.94198100
S	0.76516200	-2.02485600	1.35758500
O	1.06990800	-1.46683900	2.69092300
O	1.75341900	-1.73947900	0.28544500
C	0.87902100	-3.87277900	1.59488200
F	0.01100100	-4.28233900	2.53441000
F	2.11634500	-4.18899000	1.99063500
F	0.60758600	-4.50726600	0.45292100
C	-2.09090400	3.63559100	-0.20123600
C	-2.06830100	2.93894500	-1.41691400
C	-3.33392300	3.75822600	0.44520900
C	-3.22895400	2.38339600	-1.95952900
H	-1.14085800	2.79279700	-1.95630400
C	-4.49429600	3.20461500	-0.08867600
H	-3.41535200	4.29578800	1.38567000
C	-4.44781600	2.51311400	-1.29997100
H	-3.16570800	1.83003300	-2.89233900
H	-5.43084200	3.29963000	0.45139700
H	-5.34931900	2.06712900	-1.70978500
C	-0.95571500	5.88769900	-0.03182000
H	-1.89671900	6.24240100	0.39819000
H	-0.15613500	6.41189800	0.50939800
C	-0.85494000	6.27953300	-1.49830000
C	-1.92699700	6.50393600	-2.28902600
C	-1.79300200	6.89517300	-3.74523000
H	-2.44833100	6.26904100	-4.36547300
H	-2.12193100	7.93294300	-3.90194200
H	-0.77906100	6.80166600	-4.13787100
C	1.10641500	1.87699500	4.35575000
H	1.17760400	0.97357400	3.74555100
H	2.06983900	2.01811400	4.85520900
H	0.35439100	1.68676700	5.13233600
C	0.56165600	6.49353700	-2.02552300
H	0.65530800	7.44269600	-2.56399700
H	1.28858800	6.52164000	-1.20817200
H	0.89048900	5.70369200	-2.71454300

C	-1.09961300	1.82763500	2.42439900
H	-0.50918600	0.91984900	2.55931200
H	-1.88917300	1.79111800	3.19331100
H	-1.59389300	1.78946700	1.45530900
C	1.13895700	4.41011500	4.30795000
H	2.19665600	4.36667300	4.58716500
H	0.98277600	5.33371400	3.74906200
H	0.55549900	4.47229500	5.23515500
C	-3.37094600	6.41141600	-1.85629300
H	-3.51019800	6.36698500	-0.77557900
H	-3.92997700	7.27802900	-2.23507300
H	-3.84754800	5.51703100	-2.27862200

TS-EF-7RR-2

l imaginary frequency

H = -5472.484096

G = -5472.698681

E(M06-2X-DCM) = -5473.462225

O	-0.52782200	-2.78126000	-0.85023900
O	-2.65611300	-1.43133400	-0.19876100
P	-1.01670800	-1.35356000	-0.19667200
O	-0.60015400	-0.17946600	-1.02389900
C	-1.58574800	-3.42661900	-4.84708200
C	-2.47018200	-3.72710500	-3.81553600
C	-2.07327100	-3.58342800	-2.47940900
C	0.10714200	-2.76350700	-3.20133300
C	-0.30065700	-2.98519400	-4.52951200
C	-3.30732000	-2.46919800	0.47183900
C	-3.37729600	-3.73432600	-0.11805600
C	-3.86496200	-4.81604400	0.63365100
C	-4.37519100	-4.62477900	1.91219500
C	-4.43462400	-3.32962600	2.42388300
C	-3.91243700	-2.22997000	1.72407900
H	0.41180300	-2.78762700	-5.32512800
H	-4.89047500	-3.15033600	3.39345500
C	-3.11535500	-4.19162000	-1.55270100
C	-4.39689900	-4.03363900	-2.44038900
H	-4.78609900	-3.01655900	-2.31435300
H	-5.19048500	-4.73262800	-2.15806800
H	-4.72351500	-6.45146500	-0.50058800
H	-3.32797400	-6.92343100	0.46311900
C	-0.82843700	-3.03574900	-2.18418300
H	-1.87900400	-3.54741500	-5.88705300
H	-4.74712300	-5.46306100	2.49584000

C	-3.89792100	-4.22469200	-3.89094800
H	-4.49976300	-3.67106000	-4.62105300
H	-3.93519400	-5.28135300	-4.19110300
C	-3.74230800	-6.10909500	-0.14227400
C	-2.82192800	-5.71093000	-1.31405500
H	-1.77350700	-5.82123600	-1.01440900
H	-2.97698100	-6.31231500	-2.21538400
C	-4.15721000	-0.86348500	2.29481200
C	-3.41887500	-0.38650200	3.40218400
C	-5.26466500	-0.12334800	1.80779000
C	-2.33551400	-1.12245500	3.97825400
C	-3.76441100	0.88523300	4.00041800
C	-5.60656300	1.14069100	2.42047600
C	-1.63782200	-0.63828500	5.05272500
H	-2.05176400	-2.06489600	3.53046200
C	-3.00998100	1.35472000	5.12220900
C	-4.83860600	1.61771200	3.48717400
C	-1.97747500	0.61620700	5.63504300
H	-0.80236200	-1.20716300	5.44812000
H	-3.28571900	2.30948200	5.56503400
H	-5.10590000	2.56556000	3.95139400
H	-1.41311000	0.98186300	6.48894400
C	1.50610700	-2.30705700	-2.93246600
C	1.95759700	-1.06560600	-3.44695100
C	2.41008500	-3.16020400	-2.24968200
C	1.09259500	-0.13899100	-4.11634600
C	3.34674000	-0.69107600	-3.30083600
C	3.78534300	-2.75135100	-2.07429400
C	1.56977400	1.03447700	-4.64380200
H	0.03889100	-0.37849800	-4.19573700
C	3.80511700	0.54113900	-3.86802400
C	4.21992600	-1.53717800	-2.61227100
C	2.94737300	1.38032900	-4.52756100
H	0.89250600	1.70689500	-5.16543100
H	4.85989600	0.78842700	-3.76834900
H	5.25971400	-1.24147100	-2.49039700
H	3.31053100	2.30766600	-4.96249200
C	-7.21671600	0.10734600	0.34958200
H	-7.85292300	-0.28925700	-0.43741800
C	-6.11528700	-0.60010900	0.75779600
H	-5.88645000	-1.55242700	0.29331300
C	-7.54139000	1.35766600	0.94975300
H	-8.41883300	1.90516100	0.61568600
C	-6.75111500	1.85859800	1.95020600

H	-6.99313200	2.80709900	2.42479200
C	2.93125900	-5.23853900	-1.07368900
H	2.61402700	-6.20495200	-0.69125100
C	4.27660200	-4.81653800	-0.87925600
H	4.97137800	-5.45876000	-0.34499300
C	4.68866400	-3.60930100	-1.37289400
H	5.71575900	-3.27684500	-1.24319700
C	2.03495800	-4.44324700	-1.73768600
H	1.01922500	-4.79056000	-1.88320800
C	-1.13851600	3.92759800	-1.41669500
C	-1.11809900	4.52144700	0.03020700
H	-0.52165000	5.43002600	-0.02950000
H	-2.13016100	4.86470800	0.28236300
C	-0.60968000	3.68522600	1.17935300
C	0.27770800	3.38101000	-1.74653800
H	0.98821200	4.20403900	-1.67054900
H	0.30929500	3.02855500	-2.78185700
N	0.79725800	2.29490800	-0.90660100
C	2.02367700	2.30666300	-0.35347300
N	2.59931500	1.14007900	-0.02739700
C	3.92859800	1.00819700	0.48901000
C	5.00295500	1.24417100	-0.36593800
C	4.14470500	0.56753000	1.79505400
C	6.30642800	1.04036100	0.08554100
C	5.45571400	0.37890600	2.23786400
H	3.30108300	0.36765100	2.44708500
C	6.54051100	0.61040300	1.39058400
H	7.55264600	0.45229200	1.74206600
C	5.69452100	-0.14124700	3.63287000
C	7.44139000	1.28917700	-0.86976000
F	5.60584900	-1.48780800	3.68382300
F	4.79389900	0.35043800	4.50842300
F	6.92599900	0.19141100	4.08455800
F	7.21437400	0.68236800	-2.06630400
F	8.61737300	0.82622800	-0.40241000
F	7.59972100	2.60428700	-1.13442800
S	2.78611800	3.81374800	0.09632700
H	4.81279500	1.56263900	-1.38446500
H	2.08940800	0.25217200	-0.12121900
H	0.33474600	1.37453800	-1.01633300
C	0.41220700	4.18006100	2.01057300
H	1.39939000	3.99640600	1.09090600
N	-0.59820800	-1.44762500	1.36304100
S	0.90340100	-1.43699300	1.84840500

O	1. 13412300	-0. 46490400	2. 93541300
O	1. 91223000	-1. 45346700	0. 75663400
C	1. 10023300	-3. 10471900	2. 66512600
F	0. 87152200	-4. 08316800	1. 78685600
F	0. 23744900	-3. 22992800	3. 68716300
F	2. 34351700	-3. 22344300	3. 14102800
C	-2. 26895900	2. 92076900	-1. 69779800
C	-3. 47491600	2. 93748400	-0. 98037900
C	-2. 17862400	2. 02563100	-2. 77592700
C	-4. 53819800	2. 10089300	-1. 31725000
H	-3. 60516000	3. 60564000	-0. 13579100
C	-3. 23899400	1. 18814800	-3. 12029200
H	-1. 26828700	1. 95685900	-3. 36129700
C	-4. 42647300	1. 22156800	-2. 39252300
H	-5. 44948000	2. 13418900	-0. 72960000
H	-3. 12447600	0. 49799200	-3. 95182800
H	-5. 25134600	0. 56278500	-2. 64856300
C	-1. 29916200	5. 14948600	-2. 41847800
H	-0. 42355400	5. 79239100	-2. 28181300
H	-1. 21415000	4. 73157100	-3. 43006900
C	-2. 57410800	5. 97446600	-2. 35426400
C	-2. 65674200	7. 16812900	-1. 72498700
C	-1. 24284300	2. 35574000	1. 45278500
H	-0. 58604600	1. 65756800	1. 97347800
H	-2. 09572500	2. 53078000	2. 12991400
H	-1. 63713300	1. 87114100	0. 56204200
C	-3. 75778600	5. 42696000	-3. 14479500
H	-4. 09674100	6. 14702800	-3. 90002400
H	-3. 49334200	4. 50438500	-3. 66530000
H	-4. 61876100	5. 19058000	-2. 50988100
C	0. 84817400	3. 37413300	3. 23517100
H	1. 76766900	3. 79923100	3. 64896500
H	0. 08142500	3. 41281700	4. 01941700
H	1. 03879000	2. 32041300	3. 01879300
C	-3. 93245300	7. 98319600	-1. 70672900
H	-4. 14061900	8. 34916300	-0. 69212100
H	-3. 83230500	8. 87663300	-2. 34065000
H	-4. 80917800	7. 42996400	-2. 04708000
C	0. 64684700	5. 68365600	2. 21862800
H	0. 41228600	6. 30711300	1. 35515200
H	0. 03371700	6. 02830100	3. 06088700
H	1. 69494600	5. 86047400	2. 48123800
C	-1. 52602600	7. 87024300	-1. 00540800
H	-1. 69896300	7. 89164500	0. 08037600

H	-0.54157300	7.42970800	-1.17673300
H	-1.47407800	8.91990900	-1.32524400

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l imaginary frequency

H = -5472.484454

G = -5472.699506

E(M06-2X-DCM) = -5473.462491

O	-0.38808200	-2.72457000	-1.01651100
O	-2.52167200	-1.49729900	-0.17445700
P	-0.88587300	-1.37552900	-0.21929700
O	-0.52768900	-0.12438600	-0.95737600
C	-1.59107900	-3.04777200	-5.01240500
C	-2.42327100	-3.46652400	-3.97859200
C	-1.97666500	-3.42741700	-2.65076400
C	0.14551000	-2.47111100	-3.37964800
C	-0.30886900	-2.59070100	-4.70581700
C	-3.12127000	-2.60626600	0.42814800
C	-3.18251500	-3.81809300	-0.26547000
C	-3.61306700	-4.97317800	0.40760200
C	-4.07868000	-4.90539300	1.71536400
C	-4.14909100	-3.66082700	2.33878600
C	-3.68063700	-2.49132300	1.71833400
H	0.36334100	-2.29808600	-5.50713200
H	-4.56975600	-3.57775400	3.33681200
C	-2.96422000	-4.14470800	-1.74240200
C	-4.28385300	-3.95158400	-2.56519600
H	-4.69641000	-2.96173700	-2.33738400
H	-5.04581000	-4.69648000	-2.31514300
H	-4.47055700	-6.53160300	-0.83140600
H	-3.02766000	-7.04177800	0.03848600
C	-0.73706400	-2.86740600	-2.35568900
H	-1.92267700	-3.08750100	-6.04707500
H	-4.40713600	-5.80022400	2.23794200
C	-3.83748400	-4.00244000	-4.04411300
H	-4.48376100	-3.40922400	-4.70149200
H	-3.85503000	-5.03059300	-4.43217500
C	-3.48597300	-6.19182800	-0.48000400
C	-2.62115800	-5.66910800	-1.64534000
H	-1.55960400	-5.77296300	-1.39348900
H	-2.79416600	-6.19658100	-2.58871600
C	-3.92760200	-1.18760500	2.41973500
C	-3.16652300	-0.80992500	3.55019700
C	-5.05629200	-0.42016800	2.03415600

C	-2.05241800	-1.57622600	4.01826500
C	-3.51766900	0.38721100	4.28350700
C	-5.40216600	0.76898400	2.78008000
C	-1.33315000	-1.18833100	5.11727100
H	-1.76155200	-2.46013400	3.46729100
C	-2.74152800	0.75562300	5.42786300
C	-4.61681100	1.14740900	3.87339000
C	-1.68084300	-0.00842400	5.83494700
H	-0.47447300	-1.77469500	5.42853500
H	-3.02254700	1.65417100	5.97319200
H	-4.88879000	2.03678900	4.43952100
H	-1.09927800	0.28070900	6.70643500
C	1.53469800	-1.97909300	-3.12420200
C	1.91283300	-0.67864000	-3.54358000
C	2.49890400	-2.84491300	-2.54847300
C	0.98559300	0.26162900	-4.10163800
C	3.28840500	-0.25352400	-3.40875600
C	3.86060800	-2.38950200	-2.38303300
C	1.39060500	1.49937300	-4.53394500
H	-0.05760200	-0.02122200	-4.17756400
C	3.67174600	1.04394000	-3.87792700
C	4.22186300	-1.11426500	-2.82535400
C	2.75481400	1.89797400	-4.43009900
H	0.66539600	2.18234300	-4.97009300
H	4.71767300	1.33011800	-3.79056400
H	5.25092400	-0.78122000	-2.70955800
H	3.06111000	2.87645300	-4.79030600
C	-7.04676300	-0.07703800	0.65320200
H	-7.69688200	-0.40366300	-0.15443400
C	-5.92488000	-0.80244100	0.96080900
H	-5.69330900	-1.69855200	0.39656900
C	-7.37625000	1.09894900	1.38580500
H	-8.27246700	1.65950900	1.13243400
C	-6.56900600	1.51010100	2.41276500
H	-6.81412100	2.40026600	2.98810600
C	3.15138200	-4.98985700	-1.57541700
H	2.89014100	-5.99887500	-1.26805300
C	4.48371300	-4.52477500	-1.38974200
H	5.22460300	-5.17783600	-0.93677200
C	4.82517800	-3.26202700	-1.78948100
H	5.84115600	-2.89514700	-1.66522500
C	2.19798800	-4.18275400	-2.13785300
H	1.19329600	-4.56241300	-2.27940000
C	-1.37269700	4.04945600	-0.98103400

C	-1.32264700	4.49929600	0.51887700
H	-0.76926400	5.43783900	0.54203900
H	-2.33884900	4.74887200	0.84766100
C	-0.75199800	3.56219700	1.55448000
C	0.04382700	3.57049400	-1.40339800
H	0.73038500	4.40981000	-1.29338000
H	0.03900700	3.30037700	-2.46418300
N	0.63848500	2.44377800	-0.67179000
C	1.88559100	2.46353300	-0.16557100
N	2.52662200	1.30167900	0.02852600
C	3.88076300	1.19319600	0.48601400
C	4.90761800	1.54351200	-0.38756000
C	4.16885800	0.67240500	1.74772500
C	6.23640000	1.37401200	0.00041400
C	5.50386300	0.51939000	2.12799900
H	3.36284400	0.38180600	2.41303500
C	6.54201100	0.86483100	1.26131000
H	7.57354800	0.73390300	1.56400100
C	5.82038300	-0.08420300	3.47310800
C	7.31930400	1.74730700	-0.97450000
F	5.77159600	-1.43301800	3.43737800
F	4.94643300	0.32082600	4.41758500
F	7.06094800	0.25639700	3.89295100
F	7.08837800	1.19524900	-2.19693100
F	8.53748900	1.33497100	-0.57297300
F	7.38584900	3.08256700	-1.16773700
S	2.59278300	3.95766100	0.39983800
H	4.66185100	1.92510500	-1.37193000
H	2.05923600	0.40355400	-0.14606300
H	0.22068400	1.51151000	-0.84133500
C	0.27542100	3.99472500	2.41085100
H	1.24393400	3.96520300	1.44793600
N	-0.40990500	-1.58976400	1.31015400
S	1.10843200	-1.55516000	1.74573900
O	1.33020600	-0.68974000	2.92042800
O	2.07324300	-1.40859100	0.62556800
C	1.40823100	-3.28621000	2.37887200
F	1.19193400	-4.17989400	1.41127700
F	0.58869200	-3.55585400	3.40843000
F	2.67172800	-3.39365800	2.80105800
C	-2.49763500	3.05457400	-1.30934400
C	-3.77573100	3.20343100	-0.74254100
C	-2.33434400	2.03985500	-2.26380000
C	-4.83673000	2.37830000	-1.10817100

H	-3.96251500	3.97451700	-0.00274000
C	-3.39365800	1.20928000	-2.63349900
H	-1.36985200	1.85494700	-2.72065600
C	-4.65136300	1.37540600	-2.06073300
H	-5.80330300	2.50821300	-0.63178000
H	-3.21972600	0.41840300	-3.35770400
H	-5.47452700	0.72169200	-2.33443500
C	-1.58472000	5.34400300	-1.88161500
H	-0.73333900	6.01069200	-1.68336400
H	-1.47033600	5.00917600	-2.91597600
C	-2.86042100	6.15518100	-1.73592400
C	-3.90739400	6.04129500	-2.58313600
C	-1.35633000	2.19902100	1.69631000
H	-0.66536300	1.45316500	2.09211200
H	-2.17242200	2.27705700	2.43384700
H	-1.79492800	1.82261800	0.77377100
C	-2.86502400	7.16581900	-0.59562000
H	-3.39005100	6.80112900	0.29877400
H	-1.84331400	7.40921800	-0.28540500
H	-3.34063600	8.10911500	-0.87873600
C	0.77079100	3.06959400	3.52265800
H	1.69097900	3.47231600	3.95691400
H	0.02819900	2.99530100	4.32741200
H	0.98250700	2.05281100	3.18316000
C	-5.17959300	6.84746500	-2.43421000
H	-5.33095700	7.50052000	-3.30558000
H	-6.04715100	6.17407500	-2.40212300
H	-5.21392900	7.46758400	-1.53727700
C	0.46608300	5.47326800	2.78181400
H	0.19717000	6.17900200	1.99480200
H	-0.14276200	5.70297300	3.66527800
H	1.51266000	5.65485500	3.04700800
C	-3.97677200	5.10070200	-3.76401300
H	-4.32089700	5.64163600	-4.65622500
H	-3.03250800	4.61337300	-4.00894200
H	-4.70845200	4.30421000	-3.57414500

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l imaginary frequency

H = -5472.480949

G = -5472.693554

E(M06-2X-DCM) = -5473.453812

0	-1.54171500	-2.88905700	0.23429600
0	-2.68375200	-0.61268600	0.69834600

P	-1.21108000	-1.31332900	0.53554600
O	-0.49960700	-0.63846800	-0.60106700
C	-4.25609100	-4.05932300	-2.72912200
C	-4.69614400	-3.71167800	-1.45635400
C	-3.78235200	-3.35754900	-0.45267800
C	-1.94576200	-3.64589700	-2.03477100
C	-2.88908000	-4.04169300	-2.99919400
C	-3.44546000	-0.90712100	1.83195300
C	-4.09075100	-2.13737000	1.93645900
C	-4.60501900	-2.53214400	3.18118200
C	-4.61233400	-1.64875900	4.25593500
C	-4.13715800	-0.34891500	4.06682000
C	-3.54248700	0.05104600	2.85975700
H	-2.52921500	-4.32622500	-3.98365600
H	-4.20878000	0.37704100	4.87173600
C	-4.50539500	-3.15247700	0.87416200
C	-5.94179900	-2.79617600	0.34762200
H	-5.96696900	-1.72914600	0.09772900
H	-6.71820200	-2.98116100	1.09603900
H	-6.19652800	-4.01160200	3.16720900
H	-4.72193300	-4.57010500	3.94787400
C	-2.42473300	-3.28244100	-0.76154400
H	-4.96337500	-4.33955700	-3.50563900
H	-5.01051200	-1.94919800	5.22192300
C	-6.11383200	-3.62851000	-0.93845800
H	-6.80023600	-3.16480100	-1.65609500
H	-6.51458300	-4.62828600	-0.71804200
C	-5.09981900	-3.96327800	3.11689300
C	-4.57467200	-4.44867500	1.74401400
H	-3.56275800	-4.85459500	1.85370300
H	-5.20107800	-5.22404300	1.29093100
C	-3.15175400	1.48336600	2.65485000
C	-2.05784300	2.05405900	3.34604500
C	-3.96487900	2.29328600	1.81998000
C	-1.20121900	1.28726500	4.19768300
C	-1.76788400	3.46269900	3.19126900
C	-3.65545900	3.69667500	1.66490700
C	-0.15272600	1.86892600	4.86123800
H	-1.37751600	0.22379300	4.28970800
C	-0.66676200	4.03065700	3.90586400
C	-2.56629100	4.24198600	2.35093700
C	0.11594200	3.26035600	4.72249500
H	0.49175400	1.25779100	5.48537700
H	-0.46844300	5.09323800	3.78424200

H	-2.33626600	5.29735100	2.22574600
H	0.94933700	3.70394200	5.26139300
C	-0.49656900	-3.66373800	-2.40704000
C	-0.02637000	-2.78943600	-3.41719100
C	0.37308700	-4.62871400	-1.84214000
C	-0.83633700	-1.75171700	-3.98410600
C	1.32617200	-2.92508000	-3.90799100
C	1.73648000	-4.72335900	-2.31234200
C	-0.36949000	-0.94520700	-4.99056100
H	-1.83568300	-1.59570700	-3.59586400
C	1.76747200	-2.08074800	-4.97625000
C	2.17092600	-3.88199500	-3.34007700
C	0.94577500	-1.12285400	-5.50953500
H	-1.00489200	-0.16068800	-5.38997900
H	2.77370300	-2.22834600	-5.36390300
H	3.18945400	-3.98104700	-3.71118700
H	1.28964700	-0.49727300	-6.32960300
C	-5.88472100	2.60474100	0.33505200
H	-6.75357400	2.19509900	-0.17351000
C	-5.11697200	1.79397000	1.13004900
H	-5.38873500	0.75179700	1.25091800
C	-5.55993800	3.98044800	0.16952700
H	-6.17683400	4.60819200	-0.46799800
C	-4.47729700	4.50746400	0.82042500
H	-4.21899100	5.55633600	0.70505100
C	0.82036700	-6.47752700	-0.30868900
H	0.47723400	-7.16129000	0.46282500
C	2.16805500	-6.55230800	-0.76123000
H	2.83932100	-7.29174500	-0.33250400
C	2.60804800	-5.70078100	-1.73794600
H	3.63134300	-5.75338500	-2.10277800
C	-0.04444300	-5.55361900	-0.83263400
H	-1.06720400	-5.51488000	-0.47740600
C	5.32037900	0.88035200	0.02345300
C	5.49378300	1.53020900	-1.39932400
H	5.56429200	2.60876500	-1.24953300
H	6.47296800	1.21432300	-1.79011200
C	4.50099600	1.25667200	-2.49004300
C	4.02027200	1.43077600	0.68349100
H	4.14957100	2.50446300	0.82094000
H	3.89921200	0.97868200	1.66991700
N	2.74409500	1.23625100	-0.02349100
C	1.92686500	2.23487200	-0.45338200
N	0.63903800	1.89221900	-0.65850300

C	-0.37725800	2.65702600	-1.29459500
C	-0.63274900	3.99530800	-0.98129200
C	-1.18489400	1.99114800	-2.22330600
C	-1.65857300	4.67113400	-1.64228300
C	-2.21772100	2.67814000	-2.86114700
H	-1.01369500	0.93880800	-2.42060200
C	-2.45483100	4.02392300	-2.58669300
H	-3.26283600	4.55146800	-3.07807300
C	-3.04235600	1.96397700	-3.89856000
C	-1.87955800	6.13251400	-1.35619400
F	-2.41207700	1.94345800	-5.10452500
F	-4.23710100	2.55777300	-4.09666800
F	-3.27452600	0.67649000	-3.56518600
F	-1.59722200	6.44663800	-0.06962100
F	-3.15776100	6.50747300	-1.58993200
F	-1.09384400	6.91737600	-2.12876500
S	2.55450100	3.80403900	-0.82661400
H	-0.05409600	4.49863200	-0.22013200
H	0.34724300	0.90636600	-0.49809800
H	2.25191500	0.40232500	0.31024100
C	3.97856400	2.37221700	-3.21887200
H	3.39546200	2.86881900	-2.27242400
N	-0.53879700	-1.33939200	2.00433400
S	0.99732000	-1.65409500	2.19544500
O	1.85328600	-0.43496000	2.15153100
O	1.52520300	-2.81969100	1.46378500
C	1.02231400	-2.18261700	3.98354200
F	0.55148400	-1.23289700	4.80333200
F	2.29201600	-2.44186800	4.32476100
F	0.29639900	-3.28969900	4.14792800
C	5.44484900	-0.65021400	-0.05275200
C	6.56539100	-1.22369100	-0.68405500
C	4.48883800	-1.52172600	0.48252800
C	6.71215900	-2.60510400	-0.79053700
H	7.34751600	-0.59071900	-1.09756700
C	4.62436200	-2.91014100	0.36768500
H	3.62098200	-1.14774600	1.01058800
C	5.73464700	-3.45755800	-0.26969200
H	7.59112900	-3.01468700	-1.28225300
H	3.83908600	-3.53961800	0.77336600
H	5.84123900	-4.53513200	-0.36017000
C	6.51260800	1.47696300	0.87853300
H	6.51254000	2.55817800	0.71469200
H	7.44521700	1.10282300	0.43736900

C	6. 52776900	1. 17238800	2. 36971800
C	6. 17275900	2. 08002000	3. 30738400
C	2. 94782700	2. 13200600	-4. 32357500
H	2. 13149100	1. 47772100	-4. 00837900
H	2. 50607200	3. 08886800	-4. 61742100
H	3. 41184500	1. 69453000	-5. 21586000
C	6. 16713200	1. 77670700	4. 79110000
H	6. 94436700	2. 35552900	5. 31109800
H	5. 20911900	2. 08335700	5. 23172100
H	6. 31130900	0. 72267400	5. 03003300
C	4. 09224900	-0. 14083800	-2. 80061300
H	5. 00065200	-0. 68538600	-3. 10266700
H	3. 72658700	-0. 68352300	-1. 92574600
H	3. 36292800	-0. 21081300	-3. 60495400
C	7. 01958000	-0. 21882000	2. 73744300
H	6. 20368200	-0. 95013800	2. 79006200
H	7. 71834100	-0. 59268500	1. 98217700
H	7. 54068800	-0. 23438400	3. 69778500
C	4. 91569100	3. 54749400	-3. 58045000
H	5. 44748100	3. 30818000	-4. 50894000
H	4. 31536300	4. 44505700	-3. 75331400
H	5. 65471800	3. 78196500	-2. 81384200
C	5. 72621300	3. 50029500	3. 03320200
H	5. 89119400	3. 84269900	2. 00982400
H	4. 65584100	3. 62119300	3. 25140500
H	6. 25546500	4. 19365500	3. 70081500

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l imaginary frequency

H = -5472. 482367

G = -5472. 695601

E(M06-2X-DCM) = -5473. 455811

O	-2. 56702800	-2. 01039400	0. 04977200
O	-2. 38791600	0. 45634000	0. 83070700
P	-1. 48195000	-0. 87157300	0. 50222100
O	-0. 56046500	-0. 50127300	-0. 63356400
C	-5. 36998200	-1. 23540800	-2. 96961400
C	-5. 61183500	-0. 85245100	-1. 65505400
C	-4. 69131000	-1. 15131700	-0. 63920600
C	-3. 21303800	-2. 17312000	-2. 29011900
C	-4. 18693300	-1. 90778900	-3. 26876200
C	-3. 22327400	0. 43040700	1. 95239700
C	-4. 42963400	-0. 26694600	1. 89997900
C	-5. 13474000	-0. 50272000	3. 09081300

C	-4.72047400	0.07470800	4.28601000
C	-3.60327000	0.91052500	4.28036100
C	-2.82491100	1.09896100	3.12655000
H	-3.98876000	-2.22416500	-4.28867800
H	-3.30068400	1.41597800	5.19280800
C	-5.26245500	-0.75832600	0.71846700
C	-6.26720500	0.36440400	0.27794700
H	-5.71400200	1.30415300	0.16612200
H	-7.05789100	0.52990400	1.01587100
H	-7.26606600	-0.88078400	2.90619400
H	-6.36322000	-2.23945600	3.56626000
C	-3.48426800	-1.76731600	-0.96862400
H	-6.08705400	-1.01312500	-3.75582400
H	-5.26645800	-0.10167000	5.20941000
C	-6.79285200	-0.09083100	-1.09785100
H	-7.09406900	0.74740100	-1.73646700
H	-7.67264200	-0.74199300	-0.99523300
C	-6.31192400	-1.42181200	2.83808200
C	-6.04858200	-1.92480800	1.39987200
H	-5.40679200	-2.81263200	1.42760500
H	-6.96269300	-2.18693300	0.85734300
C	-1.67008400	2.05131300	3.17530900
C	-0.53563600	1.76584900	3.97214700
C	-1.77585100	3.30073900	2.51259700
C	-0.37030200	0.51972600	4.65579900
C	0.51236300	2.75274500	4.10858000
C	-0.71322400	4.27237300	2.64558600
C	0.72885200	0.27467300	5.43520400
H	-1.11863000	-0.24914400	4.52360700
C	1.64011300	2.46099500	4.93880400
C	0.39908200	3.97273400	3.43758000
C	1.74369400	1.26177700	5.59184100
H	0.83553800	-0.69081900	5.92042600
H	2.41191000	3.22048100	5.04275700
H	1.18912100	4.71380800	3.54427700
H	2.60179400	1.05516300	6.22633700
C	-1.96076600	-2.87732300	-2.70613200
C	-1.07076100	-2.24136800	-3.60651800
C	-1.72030200	-4.20938000	-2.29102600
C	-1.25168300	-0.89339900	-4.05903200
C	0.07742100	-2.96328800	-4.10563200
C	-0.56299900	-4.91525100	-2.79140100
C	-0.38885200	-0.31283700	-4.95333900
H	-2.09505300	-0.32393800	-3.68664200

C	0.95409200	-2.32296800	-5.03797500
C	0.30197200	-4.27591000	-3.68316800
C	0.72879700	-1.03850300	-5.45779700
H	-0.56243100	0.70837400	-5.28028600
H	1.80066100	-2.89129700	-5.41776300
H	1.16856800	-4.81496700	-4.06043500
H	1.39193900	-0.57196300	-6.18242000
C	-2.99436400	4.89768500	1.11585600
H	-3.87529300	5.15277500	0.53249700
C	-2.91699900	3.67581000	1.73206100
H	-3.73941600	2.97595600	1.63866200
C	-1.93493700	5.84125300	1.23340200
H	-2.00285200	6.79800200	0.72397500
C	-0.82983700	5.53299900	1.98020900
H	-0.01278800	6.24330300	2.07692000
C	-2.34782000	-6.21176400	-1.03973100
H	-3.02975200	-6.72240300	-0.36541500
C	-1.19899800	-6.89824900	-1.52526100
H	-1.01565400	-7.92452500	-1.21860100
C	-0.33677000	-6.26606500	-2.37938700
H	0.53768800	-6.78225400	-2.76926500
C	-2.59995900	-4.91801500	-1.41180900
H	-3.48265800	-4.41400500	-1.03640400
C	4.73067100	-1.44088700	0.05162100
C	5.50892700	-0.61028700	-1.01997100
H	5.98214100	0.21895800	-0.49672500
H	6.33327300	-1.22742600	-1.40717100
C	4.78585200	-0.06830000	-2.22131500
C	3.62691500	-0.54217600	0.67731800
H	4.12312000	0.28942500	1.17727000
H	3.06918800	-1.10014100	1.43519600
N	2.63255300	0.04314400	-0.24219900
C	2.34188500	1.37117100	-0.35368900
N	1.07422100	1.64931600	-0.70640500
C	0.50877300	2.79880700	-1.31089700
C	0.87495300	4.11977500	-1.02852600
C	-0.52773000	2.54587700	-2.22004500
C	0.23061400	5.16397200	-1.69236200
C	-1.16265300	3.60234500	-2.86827800
H	-0.82626800	1.52081000	-2.41146400
C	-0.78413500	4.92040600	-2.61719800
H	-1.28633900	5.74197100	-3.11416600
C	-2.22004400	3.30130500	-3.89686300
C	0.65290300	6.58714800	-1.43600900

F	-1.66648700	3.02474700	-5.10734400
F	-3.05918500	4.34091600	-4.08135300
F	-2.96512800	2.22729900	-3.55828700
F	1.31709000	6.72599300	-0.26897900
F	-0.40995600	7.42455900	-1.40155700
F	1.47197500	7.04244100	-2.41339500
S	3.57811800	2.56286600	-0.16155400
H	1.63149700	4.33404700	-0.28973100
H	0.40717100	0.84466700	-0.66106800
H	1.84516500	-0.57074900	-0.46083900
C	4.99218700	1.28879900	-2.58540400
H	4.37754000	1.74557800	-1.57967500
N	-0.88213300	-1.34594900	1.91221100
S	0.03452400	-2.61818300	2.15562800
O	1.35177400	-2.25076700	2.71165400
O	0.01630800	-3.61969800	1.07362600
C	-0.84804900	-3.45287000	3.57358300
F	-0.86721500	-2.67553700	4.66873300
F	-0.20802700	-4.58878100	3.87665100
F	-2.10769000	-3.74377700	3.23444700
C	4.25550300	-2.80195800	-0.48849800
C	5.13850200	-3.61287400	-1.22786100
C	2.99440700	-3.32926200	-0.18785500
C	4.76598100	-4.88264000	-1.66320700
H	6.14028700	-3.26320300	-1.46543400
C	2.61385600	-4.60218100	-0.62249500
H	2.28518700	-2.78276600	0.41833500
C	3.49644300	-5.38311000	-1.36449200
H	5.47271000	-5.48296200	-2.23092500
H	1.62415800	-4.96058000	-0.36083200
H	3.20524600	-6.37510900	-1.69954500
C	5.72451900	-1.80739000	1.23684600
H	6.50344600	-2.44515100	0.80163700
H	5.15310600	-2.46007300	1.90111300
C	6.39440600	-0.69529100	2.02913300
C	5.94028800	-0.26642200	3.22829900
C	4.29870600	1.85511900	-3.82591300
H	3.22238000	1.66433800	-3.83530100
H	4.43633100	2.93979500	-3.85817600
H	4.72616200	1.43930800	-4.74659500
C	6.64031800	0.81725600	4.01963800
H	5.92236000	1.59348600	4.31608700
H	7.05331800	0.40801200	4.95293800
H	7.45256800	1.30660200	3.47937600

C	3.89295000	-0.94765300	-3.03441600
H	4.53340800	-1.43906000	-3.78728000
H	3.41961600	-1.74176700	-2.46179300
H	3.13466200	-0.39478200	-3.58926900
C	7.68751300	-0.14211800	1.43579500
H	8.00757300	-0.73033900	0.56983600
H	7.59710000	0.90182200	1.10458700
H	8.51234200	-0.17112500	2.15679200
C	6.35613800	1.96715700	-2.35333100
H	6.99410300	1.79171500	-3.22814900
H	6.21471300	3.04742800	-2.25249300
H	6.88918400	1.61541400	-1.46989700
C	4.71598500	-0.79225700	3.94222100
H	4.24980400	-1.66361700	3.48086700
H	4.97674600	-1.06298000	4.97488000
H	3.94252500	-0.01590500	4.01536000

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1 imaginary frequency

H = -5472.484096

G = -5472.698681

E(M06-2X-DCM) = -5473.462225

O	-0.52785600	-2.78121900	-0.85028300
O	-2.65615100	-1.43130700	-0.19878100
P	-1.01674600	-1.35353100	-0.19669300
O	-0.60019700	-0.17942200	-1.02390000
C	-1.58579300	-3.42653600	-4.84713100
C	-2.47022300	-3.72703500	-3.81558600
C	-2.07330900	-3.58337000	-2.47945800
C	0.10710000	-2.76343500	-3.20138000
C	-0.30070300	-2.98511000	-4.52956000
C	-3.30735400	-2.46918100	0.47180700
C	-3.37732900	-3.73430200	-0.11810400
C	-3.86499100	-4.81602900	0.63359100
C	-4.37521800	-4.62478200	1.91213800
C	-4.43464900	-3.32963500	2.42384400
C	-3.91246500	-2.22997000	1.72405400
H	0.41175500	-2.78753300	-5.32517600
H	-4.89049700	-3.15035900	3.39342000
C	-3.11538900	-4.19157700	-1.55275500
C	-4.39693600	-4.03359000	-2.44043700
H	-4.78613800	-3.01651100	-2.31439000
H	-5.19051900	-4.73258300	-2.15812200
H	-4.72354200	-6.45143900	-0.50066900

H	-3.32799900	-6.92341300	0.46303200
C	-0.82847500	-3.03569100	-2.18423000
H	-1.87905100	-3.54732300	-5.88710300
H	-4.74714800	-5.46307200	2.49577300
C	-3.89796100	-4.22462500	-3.89100000
H	-4.49980600	-3.67098700	-4.62109700
H	-3.93523100	-5.28128200	-4.19116600
C	-3.74233500	-6.10907100	-0.14235100
C	-2.82195700	-5.71088800	-1.31412700
H	-1.77353500	-5.82119500	-1.01448400
H	-2.97700900	-6.31226400	-2.21546400
C	-4.15722600	-0.86349300	2.29481200
C	-3.41888700	-0.38654200	3.40219600
C	-5.26467100	-0.12333400	1.80780400
C	-2.33553500	-1.12251900	3.97825200
C	-3.76441200	0.88518300	4.00045700
C	-5.60656000	1.14069300	2.42052100
C	-1.63784000	-0.63838000	5.05273500
H	-2.05179400	-2.06495400	3.53044100
C	-3.00997800	1.35463800	5.12226000
C	-4.83860000	1.61768200	3.48723000
C	-1.97748100	0.61610400	5.63508000
H	-0.80238600	-1.20727500	5.44811800
H	-3.28570700	2.30939300	5.56510500
H	-5.10588800	2.56552200	3.95147200
H	-1.41311200	0.98173500	6.48898900
C	1.50606300	-2.30697800	-2.93251600
C	1.95754200	-1.06552000	-3.44699100
C	2.41005000	-3.16012600	-2.24974400
C	1.09253200	-0.13890600	-4.11637800
C	3.34668200	-0.69098000	-3.30087600
C	3.78530700	-2.75126500	-2.07436000
C	1.56969900	1.03457100	-4.64382400
H	0.03883100	-0.37842400	-4.19577400
C	3.80504700	0.54124700	-3.86804900
C	4.21987800	-1.53708300	-2.61232600
C	2.94729500	1.38043600	-4.52757700
H	0.89242500	1.70698700	-5.16544700
H	4.85982400	0.78854500	-3.76837200
H	5.25966500	-1.24137100	-2.49045600
H	3.31044400	2.30778200	-4.96249700
C	-7.21671700	0.10741300	0.34959700
H	-7.85292500	-0.28916500	-0.43741500
C	-6.11529400	-0.60006100	0.75779500

H	-5.88646300	-1.55236900	0.29328800
C	-7.54138400	1.35771800	0.94980100
H	-8.41882300	1.90522800	0.61574700
C	-6.75110700	1.85862000	1.95026800
H	-6.99311800	2.80711000	2.42487900
C	2.93124500	-5.23846800	-1.07377300
H	2.61402000	-6.20488700	-0.69134100
C	4.27658600	-4.81646100	-0.87934400
H	4.97136900	-5.45868300	-0.34509100
C	4.68863700	-3.60921600	-1.37297400
H	5.71573100	-3.27675600	-1.24328000
C	2.03493400	-4.44317500	-1.73775600
H	1.01920200	-4.79049300	-1.88327500
C	-1.13845400	3.92761900	-1.41663900
C	-1.11800300	4.52146700	0.03026300
H	-0.52150400	5.43001300	-0.02945600
H	-2.13004600	4.86478000	0.28242100
C	-0.60960800	3.68523200	1.17940900
C	0.27775600	3.38100800	-1.74650300
H	0.98827600	4.20402700	-1.67055200
H	0.30931200	3.02851900	-2.78181100
N	0.79729700	2.29491200	-0.90654500
C	2.02372600	2.30664200	-0.35343900
N	2.59933700	1.14004800	-0.02735200
C	3.92862100	1.00813700	0.48904500
C	5.00298000	1.24411800	-0.36590000
C	4.14472500	0.56743100	1.79507800
C	6.30645100	1.04028000	0.08557200
C	5.45573200	0.37878100	2.23788100
H	3.30110200	0.36754400	2.44710500
C	6.54053000	0.61028900	1.39060500
H	7.55266400	0.45215800	1.74208100
C	5.69455000	-0.14141900	3.63286700
C	7.44142100	1.28911900	-0.86971400
F	5.60606000	-1.48799600	3.68373800
F	4.79383100	0.35009400	4.50841500
F	6.92596800	0.19137700	4.08461900
F	7.21432900	0.68249600	-2.06633600
F	8.61736600	0.82599300	-0.40244200
F	7.59987800	2.60425000	-1.13420200
S	2.78621400	3.81371600	0.09631200
H	4.81282300	1.56261100	-1.38441800
H	2.08940900	0.25214900	-0.12115400
H	0.33477100	1.37455000	-1.01628400

C	0.41230500	4.18003700	2.01061900
H	1.39947000	3.99640300	1.09092800
N	-0.59824400	-1.44761600	1.36301900
S	0.90336600	-1.43703400	1.84837800
O	1.13411300	-0.46498800	2.93541900
O	1.91218900	-1.45348900	0.75660000
C	1.10017400	-3.10479300	2.66503800
F	0.87143200	-4.08320700	1.78673800
F	0.23740000	-3.23001800	3.68708100
F	2.34346100	-3.22356000	3.14092100
C	-2.26892200	2.92081700	-1.69772900
C	-3.47487700	2.93757700	-0.98030600
C	-2.17861700	2.02566100	-2.77584500
C	-4.53818300	2.10101000	-1.31716000
H	-3.60509700	3.60575100	-0.13572800
C	-3.23901300	1.18820500	-3.12019600
H	-1.26828400	1.95685100	-3.36121700
C	-4.42648700	1.22166700	-2.39242200
H	-5.44946200	2.13433800	-0.72950600
H	-3.12451700	0.49803300	-3.95172200
H	-5.25137900	0.56290300	-2.64844800
C	-1.29909100	5.14951800	-2.41841200
H	-0.42348700	5.79242400	-2.28173100
H	-1.21406500	4.73161100	-3.43000600
C	-2.57404100	5.97449400	-2.35421100
C	-2.65668900	7.16814700	-1.72491800
C	-1.24281500	2.35577100	1.45285000
H	-0.58604600	1.65758500	1.97355900
H	-2.09569700	2.53085200	2.12997000
H	-1.63711800	1.87117400	0.56211200
C	-3.75770300	5.42699500	-3.14476900
H	-4.09666100	6.14708000	-3.89998000
H	-3.49324100	4.50443800	-3.66529800
H	-4.61868000	5.19058300	-2.50986900
C	0.84828900	3.37407700	3.23519000
H	1.76779500	3.79916000	3.64897500
H	0.08155600	3.41274800	4.01945200
H	1.03889600	2.32036000	3.01878300
C	-3.93240300	7.98321100	-1.70667300
H	-4.14056100	8.34920500	-0.69207300
H	-3.83226500	8.87663100	-2.34062000
H	-4.80912900	7.42996600	-2.04700000
C	-1.52598600	7.87025800	-1.00531500
H	-1.47402700	8.91992300	-1.32515200

H	-1.69894800	7.89166300	0.08046400
H	-0.54153100	7.42971900	-1.17661700
C	0.64693800	5.68362500	2.21873200
H	1.69508200	5.86046900	2.48115200
H	0.41217300	6.30714000	1.35535300
H	0.03396000	6.02817700	3.06114000

TS-EF-7RR-7

1 imaginary frequency

H = -5472.476546

G = -5472.692777

E(M06-2X-DCM) = -5473.451246

O	-1.10125300	-2.51412600	-1.39449900
O	-2.94324100	-1.07898700	-0.26945400
P	-1.32216600	-1.26164900	-0.35928000
O	-0.77680000	0.02962500	-0.89284900
C	-2.32815100	-1.85499400	-5.34224400
C	-3.23817800	-2.26708800	-4.37401700
C	-2.80697300	-2.56895800	-3.07376500
C	-0.52315600	-1.95744500	-3.68869600
C	-0.98064900	-1.73903700	-5.00030900
C	-3.75344800	-2.13546100	0.14795900
C	-4.10343200	-3.13002100	-0.76592400
C	-4.79692100	-4.26227400	-0.30922600
C	-5.23149600	-4.34706000	1.00877600
C	-4.97094300	-3.28741600	1.87625000
C	-4.22023600	-2.16861100	1.47726400
H	-0.25626100	-1.44934000	-5.75583000
H	-5.33423100	-3.32424900	2.89895400
C	-3.94598300	-3.20538700	-2.28404000
C	-5.17563300	-2.56825500	-3.01609600
H	-5.35127000	-1.56812700	-2.60263900
H	-6.09204200	-3.15066200	-2.87917900
H	-5.98187700	-5.29977100	-1.80091900
H	-4.71828900	-6.29763300	-1.08914700
C	-1.47667000	-2.34387100	-2.72609400
H	-2.65464800	-1.63307000	-6.35523900
H	-5.77419100	-5.22076500	1.36080000
C	-4.73562700	-2.45300600	-4.49249200
H	-5.22251200	-1.62189700	-5.01572700
H	-4.98106500	-3.36458000	-5.05528800
C	-4.95133500	-5.27880800	-1.41909900
C	-3.96563100	-4.75841700	-2.48621700
H	-2.96210400	-5.15043600	-2.28510400

H	-4. 23727300	-5. 04338000	-3. 50742300
C	-4. 00267300	-1. 06353100	2. 46426500
C	-3. 26074300	-1. 30800100	3. 64641500
C	-4. 63677400	0. 18988300	2. 26985200
C	-2. 55302700	-2. 53102900	3. 87748900
C	-3. 18348000	-0. 28745600	4. 66800600
C	-4. 52303900	1. 21338800	3. 28533800
C	-1. 85343100	-2. 74237400	5. 03590800
H	-2. 54154000	-3. 28221400	3. 09868800
C	-2. 45788500	-0. 55606700	5. 87146800
C	-3. 81322100	0. 94286700	4. 45907700
C	-1. 81528800	-1. 74981100	6. 05572300
H	-1. 30192800	-3. 66843700	5. 16841200
H	-2. 42513000	0. 21727700	6. 63589600
H	-3. 75730100	1. 70656000	5. 23322100
H	-1. 26069000	-1. 93952200	6. 97079400
C	0. 93407100	-1. 80289300	-3. 38502200
C	1. 56271100	-0. 54440000	-3. 56030800
C	1. 70484100	-2. 93249300	-3. 01072500
C	0. 84354200	0. 64561300	-3. 90985800
C	2. 99281400	-0. 42684100	-3. 38018200
C	3. 12606700	-2. 78794700	-2. 79011200
C	1. 48900500	1. 83802000	-4. 11836000
H	-0. 23454700	0. 59357900	-4. 00402200
C	3. 62906700	0. 83458100	-3. 61275300
C	3. 73282600	-1. 54489900	-2. 98764400
C	2. 90372300	1. 93690600	-3. 97849000
H	0. 91671500	2. 71916400	-4. 39791500
H	4. 70951700	0. 89018600	-3. 49881000
H	4. 80534000	-1. 44279800	-2. 83410000
H	3. 39985700	2. 88618300	-4. 16232100
C	-6. 01855800	1. 71887000	0. 95245000
H	-6. 60029100	1. 92366600	0. 05837200
C	-5. 42395300	0. 49489900	1. 11304300
H	-5. 54998000	-0. 26508500	0. 35089100
C	-5. 88007000	2. 73122900	1. 94351100
H	-6. 35538400	3. 69724400	1. 79666800
C	-5. 15850500	2. 47825300	3. 07854600
H	-5. 05879700	3. 23537000	3. 85348700
C	1. 91678000	-5. 31142800	-2. 49145700
H	1. 46159200	-6. 29217800	-2. 38265400
C	3. 31031600	-5. 15583600	-2. 24721900
H	3. 90451500	-6. 01478200	-1. 94762600
C	3. 89448900	-3. 92816000	-2. 39873200

H	4.95984400	-3.79458500	-2.22699900
C	1.14551900	-4.24169700	-2.86282200
H	0.08848700	-4.38558300	-3.05285400
C	-0.86179900	4.19288800	-0.14058800
C	-1.19941300	3.69312300	1.34534100
H	-1.64819600	4.55089600	1.86028500
H	-1.99851600	2.95735000	1.24210900
C	-0.16761400	3.05883500	2.25798600
C	0.30012300	3.37175500	-0.81908200
H	1.15619700	4.02860500	-0.94664400
H	-0.01227300	3.04841900	-1.81296900
N	0.81518200	2.16902300	-0.15479600
C	2.10026500	2.01783000	0.21703500
N	2.58678200	0.77002100	0.31172800
C	3.92569800	0.42054600	0.66396700
C	4.97525900	0.80023200	-0.16953500
C	4.16172800	-0.38581200	1.77980100
C	6.27267100	0.37488400	0.11429700
C	5.46794800	-0.79088000	2.06022800
H	3.33407800	-0.70105200	2.40694500
C	6.52810400	-0.41687900	1.23204800
H	7.53691000	-0.74283600	1.45339900
C	5.72812400	-1.69572600	3.23832300
C	7.36694400	0.75370600	-0.84610000
F	5.58627400	-2.99696100	2.90654600
F	4.87827100	-1.44743200	4.25529700
F	6.98683400	-1.54380900	3.71115200
F	7.09636700	0.28883700	-2.09589000
F	8.56568500	0.25662300	-0.48540000
F	7.49541300	2.09336600	-0.95794700
S	3.03386700	3.39898000	0.72513200
H	4.76947500	1.39736700	-1.05041500
H	1.98755800	-0.04447100	0.10792800
H	0.28765800	1.30274400	-0.37292400
C	0.88460600	3.75342500	2.87685000
H	1.74696700	3.64785000	1.83303000
N	-0.86382300	-1.81002800	1.08916200
S	0.64068500	-2.13532200	1.45620100
O	1.00422500	-1.64536700	2.79595800
O	1.61280100	-1.85160400	0.36424700
C	0.66892200	-3.99857100	1.60449800
F	0.30317700	-4.56328800	0.45180800
F	-0.17100200	-4.40222900	2.56922700
F	1.90473700	-4.39930700	1.91787000

C	-2.19725600	4.02735100	-0.90178800
C	-2.52667000	2.82010400	-1.54048000
C	-3.16553800	5.04371400	-0.89088900
C	-3.75614100	2.65553100	-2.17995000
H	-1.84738200	1.97348600	-1.52365000
C	-4.39537100	4.88005700	-1.53061100
H	-2.96755400	5.98244500	-0.38797100
C	-4.69371700	3.68784500	-2.18904800
H	-3.97646100	1.70703600	-2.66212400
H	-5.11809000	5.69201500	-1.51395500
H	-5.64798700	3.56232900	-2.69414200
C	-0.41226000	5.70429700	-0.09732000
H	-0.99217200	6.19909000	0.68059200
H	0.62630000	5.71219100	0.26131300
C	-0.46799800	6.55840000	-1.36491400
C	-0.93933300	7.82677700	-1.34797200
C	-0.41896600	1.61424700	2.57631100
H	0.46998000	1.04102900	2.84338800
H	-1.08141500	1.57815600	3.45709200
H	-0.94278800	1.09421700	1.77409300
C	0.12507000	5.92565400	-2.60466600
H	0.09837600	6.57908100	-3.47598100
H	1.17333800	5.63926800	-2.44484800
H	-0.42055400	5.01399700	-2.87587300
C	1.69100000	3.06976900	3.98650500
H	2.56971500	3.67564800	4.22822000
H	1.08905600	2.97401100	4.89880500
H	2.04624000	2.07455600	3.71200400
C	-0.92774200	8.76287700	-2.53992600
H	-1.95389000	8.96524400	-2.87879200
H	-0.50273400	9.73388800	-2.25111700
H	-0.36115200	8.40324900	-3.39878300
C	-1.53899200	8.52415300	-0.14191300
H	-0.84945200	9.28893400	0.24354800
H	-2.45432700	9.05647100	-0.43320800
H	-1.79585500	7.87065900	0.69395400
C	0.84517400	5.26980900	3.07787000
H	1.83902700	5.70831000	2.93119600
H	0.14964100	5.78378900	2.41885400
H	0.54986200	5.47958000	4.11396100

TS-EF-7RR-8

l imaginary frequency

H = -5472.469623

G = -5472.685049

E(M06-2X-DCM) = -5473.446772

O	-1.82650500	-2.08668100	-1.40927000
O	-3.22623600	-0.27863900	-0.18498800
P	-1.69902400	-0.83390500	-0.35850500
O	-0.89946900	0.31441500	-0.89881200
C	-2.90468600	-1.02500500	-5.30872600
C	-3.87515600	-1.19778700	-4.32667100
C	-3.51979000	-1.64741000	-3.04644800
C	-1.17007900	-1.68422600	-3.71075500
C	-1.57206600	-1.30715800	-5.00363700
C	-4.26032500	-1.12308900	0.21770900
C	-4.87557800	-1.94815400	-0.72455000
C	-5.82597200	-2.88635800	-0.29038900
C	-6.23094900	-2.92802400	1.03911500
C	-5.68350900	-2.01768400	1.94186900
C	-4.68543100	-1.10538100	1.56111400
H	-0.81143100	-1.21586400	-5.77357300
H	-6.01599400	-2.01416400	2.97571300
C	-4.77411200	-1.98761400	-2.24898900
C	-5.79849000	-1.01396600	-2.92323500
H	-5.69134700	-0.02160800	-2.46960500
H	-6.83558700	-1.33436100	-2.78277000
H	-7.27868300	-3.49487500	-1.78084600
H	-6.30878300	-4.82723500	-1.16139400
C	-2.17306900	-1.80350200	-2.72936800
H	-3.17558300	-0.68774800	-6.30616100
H	-6.97020700	-3.65175400	1.37300500
C	-5.36830600	-0.95978800	-4.40713200
H	-5.61579400	-0.00419400	-4.88377000
H	-5.86624300	-1.74216600	-4.99680100
C	-6.27075100	-3.76714100	-1.43691800
C	-5.20842600	-3.46959300	-2.51505600
H	-4.33937700	-4.12065800	-2.36624500
H	-5.56861700	-3.62197500	-3.53719500
C	-4.17363200	-0.13435100	2.57995500
C	-3.46046300	-0.60231200	3.71062300
C	-4.50502400	1.23957800	2.46656500
C	-3.05827900	-1.96814000	3.86143200
C	-3.09572300	0.32286700	4.76051000
C	-4.10667100	2.15916000	3.50906600
C	-2.37839200	-2.39243200	4.97214600
H	-3.26484300	-2.66453700	3.05909600
C	-2.40053400	-0.16503000	5.91177300

C	-3.42437500	1.67531400	4.62948100
C	-2.05552800	-1.48449600	6.02012400
H	-2.06124400	-3.42848200	5.04454900
H	-2.14801100	0.54251200	6.69855600
H	-3.15253900	2.36751100	5.42480000
H	-1.52102500	-1.84221600	6.89603000
C	0.26874200	-1.98621900	-3.43190200
C	1.24840200	-0.97061000	-3.55476000
C	0.65879800	-3.31304900	-3.11870700
C	0.92390700	0.39081300	-3.86335400
C	2.64517700	-1.29549700	-3.36498300
C	2.05447200	-3.61460200	-2.89767600
C	1.90091000	1.33991700	-4.02177200
H	-0.11887000	0.66685300	-3.96649200
C	3.63336500	-0.27324000	-3.53147400
C	3.00758300	-2.60182000	-3.02969500
C	3.27709300	1.00736000	-3.86035600
H	1.62396000	2.36010700	-4.27381600
H	4.67882900	-0.54059200	-3.39308500
H	4.05859900	-2.83911500	-2.87782200
H	4.03676000	1.77241300	-3.99764700
C	-5.55805200	3.10669000	1.28843500
H	-6.12513800	3.48205000	0.44118700
C	-5.25519400	1.77259800	1.36905500
H	-5.59277700	1.09848700	0.59033600
C	-5.13944200	4.01119100	2.30495400
H	-5.38542600	5.06629600	2.22190600
C	-4.43955000	3.54484500	3.38457700
H	-4.12789100	4.22084600	4.17796600
C	0.13988400	-5.66967100	-2.72787000
H	-0.59013900	-6.47266400	-2.67038300
C	1.51284700	-5.95351700	-2.48284000
H	1.81820500	-6.96592500	-2.23299500
C	2.44047200	-4.95178100	-2.57113300
H	3.49460200	-5.15380400	-2.39679900
C	-0.27005800	-4.39908300	-3.03613200
H	-1.31939600	-4.20794000	-3.22809900
C	0.13445400	4.27576900	-0.05782200
C	-0.31395200	3.83040400	1.41474500
H	-0.52557000	4.76506800	1.94866400
H	-1.27448400	3.32489100	1.30750800
C	0.53809000	2.93519900	2.29173000
C	0.89906900	3.14914300	-0.85828200
H	1.82193500	3.57990400	-1.24550900

H	0.29809400	2.83490700	-1.71109000
N	1.25029800	1.89347400	-0.18101500
C	2.49590400	1.51468500	0.15168400
N	2.74399100	0.19583800	0.24184000
C	3.97980400	-0.40679400	0.61613300
C	5.13571700	-0.15464500	-0.12353700
C	4.00008800	-1.32135100	1.67219700
C	6.32286400	-0.80606900	0.20733300
C	5.19735800	-1.96552900	1.99167700
H	3.09163000	-1.52782500	2.22956600
C	6.36242700	-1.71119700	1.26769700
H	7.28556000	-2.21808500	1.52094600
C	5.21474700	-2.99050600	3.09778100
C	7.56448200	-0.50233500	-0.58840000
F	4.85468900	-4.21201100	2.64750000
F	4.36464300	-2.66513000	4.09237500
F	6.44821000	-3.11655800	3.63891600
F	7.28170400	-0.36067500	-1.90654900
F	8.48990400	-1.47750800	-0.47483300
F	8.14720400	0.65000800	-0.19026500
S	3.67143100	2.70962100	0.62327600
H	5.09584200	0.52121300	-0.96896800
H	1.98545500	-0.48289200	0.06464800
H	0.55602100	1.14533400	-0.36190200
C	1.72945700	3.33448700	2.91862500
H	2.51574600	3.13574900	1.81386100
N	-1.31010400	-1.50860900	1.05829000
S	0.09720700	-2.16975400	1.34802900
O	0.60921700	-1.82596400	2.68498400
O	1.07324800	-2.06105800	0.22640600
C	-0.27537700	-3.99968400	1.43908900
F	-0.79475300	-4.42845700	0.28776300
F	-1.14879400	-4.24588400	2.42647000
F	0.85422700	-4.66869500	1.68935000
C	-1.20851500	4.63862600	-0.73367200
C	-2.07868700	3.61854300	-1.15739700
C	-1.63810300	5.96629800	-0.87068600
C	-3.31885800	3.91981600	-1.71884300
H	-1.80084400	2.57263300	-1.04749800
C	-2.88120500	6.26798800	-1.43197400
H	-0.99364800	6.78514200	-0.57128000
C	-3.72702000	5.24699100	-1.86181200
H	-3.96619300	3.10773000	-2.03789400
H	-3.18187100	7.30747500	-1.53577100

H	-4.69225000	5.48216000	-2.30259400
C	1.09005300	5.49347800	0.08323200
H	0.58648300	6.24055200	0.71302600
H	1.92370500	5.13652400	0.69670500
C	1.78538700	6.27699600	-1.03853500
C	1.70863000	6.22937300	-2.38562600
C	-0.04827200	1.58131700	2.55673000
H	0.67409700	0.80411500	2.80779900
H	-0.70773200	1.67961900	3.43564100
H	-0.67588000	1.22761800	1.73928200
C	2.77371700	7.24670000	-0.39272500
H	3.78130100	6.81091700	-0.32842800
H	2.85884700	8.18901600	-0.94014100
H	2.47270800	7.49508900	0.63128900
C	2.40136600	2.40009100	3.92985800
H	3.39637700	2.78285700	4.17744400
H	1.82074700	2.35184400	4.85958100
H	2.52690100	1.38080100	3.55876200
C	2.61336500	7.11589100	-3.23413800
H	3.63839600	7.16823200	-2.85487000
H	2.66378200	6.73964500	-4.26138500
H	2.23356000	8.14620400	-3.29265200
C	0.79974400	5.38611000	-3.24609500
H	0.25960100	6.03267300	-3.95196400
H	1.39312700	4.69362200	-3.86034300
H	0.05216400	4.81524400	-2.70548300
C	2.02043200	4.80185800	3.25206400
H	3.05549400	5.06877600	3.00829000
H	1.35983900	5.50837600	2.75260100
H	1.90031900	4.93752400	4.33428300

TS-EF-7RR-9

l imaginary frequency

H = -5472.469794

G = -5472.684975

E(M06-2X-DCM) = -5473.449508

O	-0.22562100	-2.88499500	-0.97721800
O	-2.38190700	-1.72692200	-0.12778700
P	-0.74648200	-1.56425800	-0.15630500
O	-0.44533900	-0.28497100	-0.87436600
C	-1.46196700	-3.24430100	-4.96222300
C	-2.26702400	-3.69832200	-3.92250200
C	-1.81563000	-3.64199000	-2.59597200
C	0.25574900	-2.58792300	-3.34252300

C	-0.20219200	-2.72512500	-4.66524100
C	-2.95540900	-2.84480500	0.48444600
C	-3.01231300	-4.05477600	-0.20937100
C	-3.42730100	-5.21249100	0.46854400
C	-3.89097500	-5.14370700	1.77722800
C	-3.94822100	-3.90220100	2.40823000
C	-3.47631400	-2.73248400	1.78933700
H	0.44697900	-2.39312200	-5.47003900
H	-4.34714100	-3.82527500	3.41532800
C	-2.78292400	-4.38526000	-1.68325400
C	-4.10822200	-4.23635300	-2.50656400
H	-4.55238200	-3.25819600	-2.28644800
H	-4.84805900	-5.00094600	-2.25022000
H	-4.24841000	-6.79210800	-0.77147300
H	-2.80527600	-7.27218400	0.11479400
C	-0.59508400	-3.03302700	-2.31239700
H	-1.80093200	-3.29706300	-5.99387500
H	-4.21637200	-6.03903500	2.30090100
C	-3.66068700	-4.28478400	-3.98399700
H	-4.32688200	-3.72077800	-4.64710300
H	-3.64216700	-5.31666700	-4.36205000
C	-3.27353600	-6.43315100	-0.41239200
C	-2.40625100	-5.90058000	-1.57266200
H	-1.34551400	-5.97974500	-1.30887500
H	-2.55822800	-6.43835700	-2.51378800
C	-3.61688000	-1.43624900	2.52628900
C	-2.90562200	-1.22479100	3.73288600
C	-4.56606400	-0.47985500	2.08380600
C	-1.90392100	-2.13081300	4.20759000
C	-3.17398400	-0.04541000	4.52602900
C	-4.80372900	0.70925000	2.87206700
C	-1.23893900	-1.90433900	5.38324400
H	-1.64245300	-2.98529000	3.59772600
C	-2.46996200	0.14341700	5.75703100
C	-4.11185400	0.88792300	4.07414500
C	-1.53290200	-0.76042000	6.17813600
H	-0.46050200	-2.59206200	5.69949700
H	-2.69513100	1.02823400	6.34846600
H	-4.31699500	1.77026700	4.67828300
H	-0.99842700	-0.60221600	7.11098900
C	1.61484200	-2.01279100	-3.09951800
C	1.90060300	-0.68735500	-3.51367100
C	2.64098800	-2.81959700	-2.54700800
C	0.90113000	0.20000400	-4.03287700

C	3.25057600	-0.18038100	-3.40847000
C	3.97385600	-2.27971500	-2.40188500
C	1.22040200	1.46111900	-4.46866800
H	-0.12879800	-0.13470900	-4.06615700
C	3.54369000	1.13832300	-3.88343900
C	4.24661200	-0.98337500	-2.84628800
C	2.56204100	1.93721000	-4.40655400
H	0.44101900	2.10427400	-4.87015600
H	4.57212300	1.48717100	-3.82133400
H	5.25450200	-0.58646900	-2.74670000
H	2.79982000	2.93312700	-4.77099000
C	-6.25551600	0.29499200	0.49206000
H	-6.82677300	0.14088900	-0.41916900
C	-5.34377100	-0.64679900	0.89257800
H	-5.20798700	-1.54552700	0.30217900
C	-6.46798300	1.47436400	1.26075700
H	-7.19813700	2.20851200	0.93110300
C	-5.76341000	1.66861700	2.41870700
H	-5.92963000	2.55515200	3.02707400
C	3.44309100	-4.92369800	-1.59719000
H	3.25110400	-5.94848100	-1.29085200
C	4.74639200	-4.37611100	-1.43057400
H	5.53432200	-4.98313400	-0.99317600
C	5.00098400	-3.09246000	-1.82871300
H	5.99377000	-2.66281400	-1.71878900
C	2.43159900	-4.17586100	-2.13976100
H	1.45009800	-4.61691300	-2.26626300
C	-1.88007600	3.81203300	-1.14635500
C	-2.20759900	3.66244000	0.40981900
H	-2.70901200	4.58636700	0.70800000
H	-2.94635700	2.86642100	0.51770100
C	-1.12533000	3.36568000	1.42668900
C	-0.38117100	3.48282200	-1.51163400
H	0.22601600	4.37824700	-1.38808800
H	-0.35434500	3.20754900	-2.57144200
N	0.30279400	2.42488200	-0.76856200
C	1.54979800	2.56244700	-0.27153800
N	2.25994600	1.45373500	-0.00927500
C	3.61768100	1.45934300	0.45122400
C	4.62378500	1.84039200	-0.43370200
C	3.93219600	1.02241700	1.73793900
C	5.95778600	1.78803400	-0.02986200
C	5.27114000	0.98404300	2.13247200
H	3.14606600	0.69916000	2.41189500

C	6.28858700	1.36314600	1.25582500
H	7.32408700	1.32226500	1.56986000
C	5.61311300	0.47095700	3.50852900
C	7.02052700	2.19670700	-1.01288000
F	5.59482400	-0.87740800	3.55600800
F	4.73589900	0.91373000	4.43374700
F	6.84767800	0.86632800	3.89692100
F	6.85270900	1.56751300	-2.20786900
F	8.26232400	1.90506700	-0.57883200
F	6.98252000	3.52177100	-1.27366500
S	2.16869800	4.13141900	0.16553300
H	4.35968100	2.15400300	-1.43717300
H	1.85163100	0.52357100	-0.15809900
H	-0.01512600	1.45405100	-0.92582600
C	-0.29092300	4.35889500	1.97705800
H	0.69315200	4.25873900	1.09064800
N	-0.27504600	-1.78128200	1.37027500
S	1.23678400	-1.61048200	1.81883600
O	1.36426500	-0.77770000	3.02735700
O	2.17543500	-1.32039600	0.70626900
C	1.70124400	-3.33190000	2.37561000
F	1.58652700	-4.19411600	1.36228000
F	0.90295200	-3.73412100	3.37729700
F	2.96499000	-3.33268100	2.81067400
C	-2.76238400	2.88383600	-2.01542100
C	-2.92876600	1.53244400	-1.68281700
C	-3.32837900	3.32818600	-3.22315300
C	-3.62277800	0.65634300	-2.51851000
H	-2.49883800	1.12528900	-0.77661800
C	-4.03197000	2.45760700	-4.05643100
H	-3.25381500	4.36879200	-3.51638400
C	-4.17958500	1.11430200	-3.71129700
H	-3.70779000	-0.38538500	-2.22612900
H	-4.46623400	2.83719600	-4.97789900
H	-4.72159900	0.43521500	-4.36406400
C	-2.00361000	5.31001100	-1.56347500
H	-1.18927400	5.82979700	-1.03991600
H	-1.69693500	5.37535400	-2.61753200
C	-3.21052000	6.23888400	-1.39434600
C	-4.46877300	6.02688100	-0.95133500
C	-1.08094700	1.96141900	1.94636600
H	-0.10160900	1.64180400	2.30748000
H	-1.76058500	1.90126700	2.81227000
H	-1.43515700	1.23340400	1.21683000

C	-2.78416500	7.65395800	-1.78972800
H	-3.56417100	8.18732500	-2.33983200
H	-2.52461700	8.26537800	-0.91348300
H	-1.89642800	7.63284600	-2.43086900
C	0.47319000	4.06348000	3.27417000
H	1.21640300	4.84711000	3.44944600
H	-0.21466800	4.05532700	4.12887900
H	1.00174600	3.10880300	3.25854700
C	-5.44489100	7.18484400	-0.80530200
H	-6.05670600	7.30518100	-1.71161100
H	-6.14344000	6.98731200	0.01639300
H	-4.96311500	8.14382400	-0.60215200
C	-5.11859800	4.71855400	-0.56734300
H	-5.33277100	4.69106100	0.51063400
H	-6.09092700	4.63638000	-1.07298900
H	-4.55167300	3.83029800	-0.82655600
C	-0.63957800	5.84537700	1.86267600
H	0.27575000	6.44696500	1.84668000
H	-1.22137100	6.09636200	0.97689200
H	-1.21616000	6.15382600	2.74427600

TS-1-1-7SS

l imaginary frequency

H = -5472.465669

G = -5472.676918

E(M06-2X-DCM) = -5473.443208

C	-3.44005500	2.16587100	1.96348700
C	-3.00350900	1.29473600	3.22446700
H	-3.87260300	0.69998200	3.49943300
H	-2.84580200	2.02129600	4.03390800
C	-1.78022500	0.42390100	3.25248000
C	-2.35845900	3.20805700	1.59369600
H	-2.78745800	3.95006800	0.91832700
H	-2.06437100	3.76147700	2.49395000
N	-1.15287900	2.68227200	0.96720600
C	-0.10891700	3.49563600	0.63658500
N	0.96675800	2.79233800	0.14650900
C	2.19692600	3.23620900	-0.36056400
C	2.84763400	4.41193700	0.04232100
C	2.82495000	2.39997700	-1.30047100
C	4.08813300	4.73986200	-0.50765200
C	4.06072300	2.74821100	-1.83992600
H	2.32087400	1.49743600	-1.62955000
C	4.70570600	3.92416300	-1.45291900

H	5. 65787500	4. 20315600	-1. 88672300
C	4. 72699900	1. 83790700	-2. 83367400
C	4. 79594200	5. 97229100	-0. 00562600
F	3. 82628400	1. 10832900	-3. 54259100
F	5. 47712200	2. 51983300	-3. 72289700
F	5. 55327400	0. 94526700	-2. 23131200
F	5. 72826800	6. 41142300	-0. 88011100
F	3. 94064300	6. 98873400	0. 22374200
F	5. 43687800	5. 72704400	1. 16341000
S	-0. 19575900	5. 16966200	0. 82338300
H	2. 37589200	5. 06873600	0. 75902900
C	-1. 85400200	-0. 98500900	3. 21948100
H	0. 84106000	1. 77822600	0. 09419600
H	-1. 02545900	1. 68162900	0. 85227300
H	-1. 61593600	-1. 23032700	1. 93967500
O	1. 27216600	-2. 46749600	0. 38849100
O	0. 24068300	-1. 07700800	-1. 57188200
P	0. 18352200	-1. 31202500	0. 03311500
O	0. 45198800	0. 02183300	0. 65608400
C	5. 34580800	-1. 66872900	-0. 25915700
C	4. 53356500	-2. 10167300	-1. 29965200
C	3. 18724300	-2. 43409800	-1. 07253200
C	3. 45617800	-1. 86321300	1. 28459400
C	4. 81002300	-1. 58781500	1. 02293300
C	0. 16081600	-2. 00724000	-2. 62420000
C	1. 14201700	-2. 98570400	-2. 77917900
C	0. 89885800	-4. 05087000	-3. 66296700
C	-0. 20029100	-4. 03267000	-4. 51157900
C	-1. 04296100	-2. 92450000	-4. 49096700
C	-0. 90190100	-1. 89463400	-3. 54413400
H	5. 44156700	-1. 29256600	1. 85529800
H	-1. 85393500	-2. 85134200	-5. 20810200
C	2. 59739600	-3. 06945400	-2. 32357600
C	3. 51219500	-2. 41401700	-3. 41925700
H	3. 52436000	-2. 98898900	-4. 34918200
H	3. 12719500	-1. 41494900	-3. 64995500
H	2. 60315100	-5. 13544500	-4. 46381600
H	1. 57509500	-6. 10480800	-3. 41579200
C	2. 64644600	-2. 24076900	0. 19563000
H	6. 38532400	-1. 40767700	-0. 43683900
H	-0. 37968700	-4. 84491000	-5. 21129200
C	4. 89479600	-2. 28199000	-2. 75482300
H	5. 47256100	-1. 43815100	-3. 14315100
H	5. 50287300	-3. 18547200	-2. 90218800

C	1. 98665500	-5. 09845900	-3. 55538700
C	2. 80289400	-4. 61866500	-2. 33521600
H	2. 38070100	-5. 03666400	-1. 41387300
H	3. 85943800	-4. 90035100	-2. 37995400
C	-1. 82358800	-0. 72111300	-3. 64660500
C	-3. 22926000	-0. 92405400	-3. 64494000
C	-1. 29406100	0. 56461000	-3. 94079600
C	-3. 83616800	-2. 18331900	-3. 32532600
C	-4. 10957500	0. 16836200	-3. 99256500
C	-2. 19475900	1. 66360900	-4. 20969200
C	-5. 19249200	-2. 36406200	-3. 41176800
H	-3. 20754100	-2. 99708700	-2. 98801700
C	-5. 51638700	-0. 06890400	-4. 09012900
C	-3. 57191400	1. 43175500	-4. 24691300
C	-6. 04688100	-1. 30173100	-3. 82143700
H	-5. 62183800	-3. 32954600	-3. 15833500
H	-6. 15535600	0. 75836900	-4. 38948300
H	-4. 24044300	2. 25299200	-4. 49746600
H	-7. 11699500	-1. 47132000	-3. 90830200
C	3. 01370400	-1. 80386800	2. 71296200
C	3. 05044800	-0. 56788100	3. 40571700
C	2. 72823000	-3. 00403600	3. 41218100
C	3. 29382000	0. 68200800	2. 74720200
C	2. 82992900	-0. 54096500	4. 83477700
C	2. 49230300	-2. 95899100	4. 83837700
C	3. 33978300	1. 86070800	3. 44620400
H	3. 42932300	0. 68840100	1. 67212400
C	2. 89174500	0. 71008900	5. 52692200
C	2. 56196500	-1. 73472100	5. 51032400
C	3. 14393100	1. 87759900	4. 85713800
H	3. 52259200	2. 79289800	2. 91907600
H	2. 73692300	0. 71019700	6. 60354200
H	2. 40450500	-1. 71153400	6. 58699500
H	3. 19161100	2. 82050000	5. 39484200
C	0. 58337500	2. 08992600	-4. 32546900
H	1. 65457400	2. 25108000	-4. 39621100
C	0. 10891100	0. 83487500	-4. 04379500
H	0. 81326100	0. 02237000	-3. 91379400
C	-0. 31070700	3. 17776000	-4. 53138600
H	0. 08277600	4. 16868100	-4. 73948100
C	-1. 66068600	2. 96243700	-4. 48274600
H	-2. 35932100	3. 77646000	-4. 66097900
C	2. 40497600	-5. 42589800	3. 48186900
H	2. 37476000	-6. 38371300	2. 96974400

C	2. 15748600	-5. 37289600	4. 88294300
H	1. 93779400	-6. 28783400	5. 42619300
C	2. 20583500	-4. 17274200	5. 53872600
H	2. 02893400	-4. 11817400	6. 61036300
C	2. 68616800	-4. 28580600	2. 77515600
H	2. 88239600	-4. 35041100	1. 71153400
N	-1. 23349900	-1. 91214400	0. 65459700
S	-2. 08737500	-3. 22387900	0. 18598600
C	-1. 43483400	-4. 69594600	1. 15906300
O	-3. 46286800	-3. 05981200	0. 65548600
O	-1. 79943900	-3. 60905100	-1. 19660200
F	-2. 08638000	-5. 78131400	0. 73660900
F	-1. 66054800	-4. 55376800	2. 47608800
F	-0. 12735200	-4. 86452900	0. 96158200
C	-0. 47398600	1. 10219300	3. 52241600
H	0. 31439100	0. 75492100	2. 84913600
H	-0. 54489400	2. 18762200	3. 46110000
H	-0. 14954700	0. 83448600	4. 53930900
C	-0. 67593700	-1. 74657900	3. 84283300
H	-0. 69140400	-1. 63083800	4. 93441500
H	-0. 74883100	-2. 80945200	3. 61837500
H	0. 28924600	-1. 39531400	3. 48041000
C	-4. 69313800	2. 91686900	2. 48446400
C	-5. 85334500	2. 18728200	2. 79660200
C	-4. 71992900	4. 30016700	2. 71758100
C	-6. 98851700	2. 80597900	3. 31464500
H	-5. 88026700	1. 11557100	2. 62733700
C	-5. 85915900	4. 92540400	3. 23446700
H	-3. 85879200	4. 92136900	2. 50040300
C	-6. 99810800	4. 18427000	3. 53675400
H	-7. 86801000	2. 20875400	3. 54078900
H	-5. 84498700	5. 99936500	3. 39993400
H	-7. 88206300	4. 67116000	3. 93944700
C	-3. 80307300	1. 21274200	0. 75833600
H	-4. 12970500	0. 25969300	1. 17220100
H	-2. 87993500	0. 98771500	0. 20739500
C	-4. 84859000	1. 73547100	-0. 21536800
C	-6. 02158500	1. 10024100	-0. 43007800
C	-4. 47052300	3. 01801700	-0. 93046100
H	-3. 40092300	3. 02134100	-1. 17033200
H	-5. 00444900	3. 14385300	-1. 87390900
H	-4. 66968300	3. 90927100	-0. 31985600
C	-7. 13649300	1. 67589900	-1. 27589200
H	-6. 95078300	2. 69129700	-1. 62883800

H	-7.33966300	1.03850600	-2.14588600
H	-8.06376300	1.70282900	-0.68578200
C	-3.20807000	-1.67045900	3.46507600
H	-3.53165200	-1.49968300	4.50036200
H	-3.99535100	-1.33221600	2.79079000
H	-3.11096200	-2.74553300	3.31753100
C	-6.40748700	-0.24411000	0.15180200
H	-6.88922600	-0.85002600	-0.62576700
H	-5.57091100	-0.83632600	0.52805100
H	-7.14741600	-0.13400300	0.95892200

TS-1-1-7SS-1

l imaginary frequency

H = -5472.460797

G = -5472.672902

E(M06-2X-DCM) = -5473.441397

C	3.94945300	0.84878500	-2.14988000
C	3.46206200	-0.38387400	-3.02915500
H	4.17046900	-1.18745800	-2.84896700
H	3.61872500	-0.06173200	-4.07183300
C	2.07864300	-0.96521000	-3.08872500
C	3.05358700	2.09593900	-2.30235000
H	3.54385700	2.93254900	-1.79794200
H	2.97894000	2.37699000	-3.36027300
N	1.71418700	1.97075100	-1.74764100
C	0.88565400	3.04061200	-1.61187600
N	-0.26876300	2.72524700	-0.92895600
C	-1.24500100	3.57976900	-0.38600400
C	-1.72637400	4.72775400	-1.02869100
C	-1.78093400	3.21741000	0.86178600
C	-2.71212200	5.50318800	-0.41379900
C	-2.76265500	4.00324900	1.45755800
H	-1.40136400	2.33891900	1.37293800
C	-3.23618600	5.15701700	0.82874300
H	-3.98870600	5.77682500	1.30243100
C	-3.31775900	3.64847500	2.80865300
C	-3.26629400	6.69667900	-1.14900600
F	-2.72151500	2.55573800	3.34526800
F	-3.16465700	4.65639900	3.69469200
F	-4.64786900	3.38514400	2.75201400
F	-3.78006600	7.61524000	-0.30065500
F	-2.32792300	7.31069500	-1.89693200
F	-4.26624600	6.33613900	-1.98940800
S	1.28520800	4.56520000	-2.21229200

H	-1.31730900	5.02196900	-1.98461100
C	1.82218800	-2.31686100	-2.76409900
H	-0.34215100	1.75258700	-0.62132200
H	1.41787500	1.09530300	-1.32586000
H	1.36187900	-2.22494300	-1.54171500
O	-1.85601300	-2.09880000	-0.08822600
O	-0.42557500	-0.80411900	1.67952100
P	-0.42691100	-1.35588300	0.14700100
O	-0.17759600	-0.15890600	-0.71787400
C	-5.36508500	0.19231400	0.13117000
C	-4.76686500	-0.29965300	1.28556900
C	-3.63371700	-1.12634300	1.21034700
C	-3.68271100	-0.95815800	-1.22470000
C	-4.84140600	-0.17085900	-1.10789500
C	-0.67098700	-1.53665500	2.85672300
C	-1.93535900	-2.07001200	3.10475700
C	-2.07795600	-3.01775000	4.13130500
C	-1.02648800	-3.29464500	4.99585900
C	0.16095800	-2.58013000	4.85569700
C	0.37305600	-1.69071100	3.78938100
H	-5.32919100	0.16094900	-2.01959500
H	0.96384000	-2.71643200	5.57385300
C	-3.32340300	-1.70822500	2.58200700
C	-3.95386300	-0.60436300	3.50198200
H	-4.20171000	-0.98668900	4.49613500
H	-3.23080100	0.20641400	3.62870300
H	-4.05195500	-3.27904300	5.00003700
H	-3.45479100	-4.70361200	4.15681200
C	-3.05884900	-1.37587000	-0.03237300
H	-6.24174300	0.83208800	0.18829800
H	-1.13654100	-4.02491800	5.79335300
C	-5.17611700	-0.07881700	2.72345800
H	-5.38725600	0.97348900	2.93766400
H	-6.08611500	-0.64570400	2.96484000
C	-3.47211400	-3.60814400	4.12684400
C	-4.07007900	-3.06235100	2.81139300
H	-3.83383300	-3.74131800	1.98397000
H	-5.15700200	-2.93744700	2.84555600
C	1.63830000	-0.88629400	3.80416000
C	2.89534900	-1.51770300	3.64208600
C	1.57264000	0.48048400	4.18117900
C	3.02437700	-2.89097900	3.25869100
C	4.11014000	-0.76648300	3.86727200
C	2.79577700	1.20909800	4.43372500

C	4. 25496000	-3. 47180700	3. 09382400
H	2. 12777200	-3. 47190500	3. 08286800
C	5. 37344800	-1. 41327200	3. 69291100
C	4. 02665100	0. 56824200	4. 26979100
C	5. 44787300	-2. 72718800	3. 31557500
H	4. 31770900	-4. 50902800	2. 77812000
H	6. 27636800	-0. 83296700	3. 86877900
H	4. 94301000	1. 12117700	4. 46658800
H	6. 41455400	-3. 20624900	3. 18378000
C	-3. 25480400	-1. 37527400	-2. 59787800
C	-2. 80181800	-0. 40663500	-3. 52695900
C	-3. 45860400	-2. 71673700	-3. 01144200
C	-2. 58274800	0. 96446100	-3. 17230200
C	-2. 54537600	-0. 79300800	-4. 89734300
C	-3. 17359800	-3. 09373700	-4. 37825800
C	-2. 16672300	1. 88475900	-4. 09962600
H	-2. 74448800	1. 27050300	-2. 14569100
C	-2. 11391900	0. 19928400	-5. 83367000
C	-2. 72861000	-2. 12399700	-5. 28156700
C	-1. 93428300	1. 50189700	-5. 45172700
H	-2. 00494900	2. 91623200	-3. 80103500
H	-1. 93850300	-0. 10689800	-6. 86257800
H	-2. 53545400	-2. 41004200	-6. 31374500
H	-1. 61147400	2. 24757500	-6. 17295100
C	0. 31022400	2. 49721000	4. 76169300
H	-0. 64383400	3. 00226400	4. 87874200
C	0. 33841200	1. 18387000	4. 36893700
H	-0. 59508900	0. 65966800	4. 20189600
C	1. 51875000	3. 20421100	5. 01874200
H	1. 47882800	4. 24119500	5. 34072600
C	2. 72292800	2. 57226500	4. 86257800
H	3. 65431100	3. 09780800	5. 06097900
C	-4. 17516000	-5. 01347200	-2. 57810600
H	-4. 57357100	-5. 75921000	-1. 89560200
C	-3. 86348600	-5. 38518800	-3. 91647500
H	-4. 02037400	-6. 41000100	-4. 24154700
C	-3. 37988300	-4. 44821900	-4. 78866600
H	-3. 15160100	-4. 71346300	-5. 81832600
C	-3. 98195400	-3. 72838600	-2. 14343100
H	-4. 23326900	-3. 46509900	-1. 12261500
N	0. 68413900	-2. 52876300	-0. 22485500
S	0. 85105700	-4. 00753300	0. 46058400
C	-0. 11907300	-5. 23215200	-0. 60373200
O	2. 23962500	-4. 44126700	0. 31282300

O	0.16917600	-4.08873000	1.75428300
F	-0.44601400	-6.27384800	0.16097500
F	0.64056600	-5.67692700	-1.61980100
F	-1.22596600	-4.68424300	-1.10291100
C	1.01304200	-0.15205700	-3.75074600
H	0.10073100	-0.12130100	-3.14775600
H	1.32688900	0.86781300	-3.96239400
H	0.73897600	-0.63794200	-4.69782100
C	0.61260000	-2.95812700	-3.46657200
H	0.79028400	-3.01117700	-4.54898600
H	0.45953100	-3.97400700	-3.10913300
H	-0.31309800	-2.40361800	-3.30500300
C	5.34998400	1.17394500	-2.74311300
C	6.33319300	0.16987600	-2.80961300
C	5.69151700	2.43618100	-3.25299500
C	7.59092800	0.40877900	-3.35900800
H	6.13278000	-0.81880300	-2.40751900
C	6.95381500	2.68129900	-3.80154000
H	4.98543100	3.25727600	-3.23120000
C	7.90988600	1.67076600	-3.86181800
H	8.32346900	-0.39358600	-3.38715900
H	7.18117200	3.67293100	-4.18353900
H	8.88964000	1.86219500	-4.29063300
C	4.08131600	0.43152400	-0.63437100
H	4.52581500	-0.57033900	-0.60274100
H	3.07537400	0.31402700	-0.21730200
C	4.92704400	1.36189700	0.23326800
C	4.42834400	2.40035600	0.93952900
C	6.41242000	1.02888200	0.30514400
H	6.59022500	-0.01785400	0.04143800
H	7.02392200	1.63453800	-0.37511100
H	6.80488400	1.17177000	1.31669300
C	5.32348800	3.35132000	1.70841400
H	6.36779500	3.32713000	1.39129700
H	4.96376800	4.38092200	1.58625700
H	5.28979300	3.13849800	2.78677900
C	3.00683700	-3.28027100	-2.57027500
H	3.56612200	-3.39616000	-3.50765300
H	3.69403600	-2.95656800	-1.78574500
H	2.63891900	-4.26185200	-2.27341900
C	2.96771900	2.75147600	1.08821400
H	2.69543500	3.61338100	0.46409800
H	2.29345400	1.92956000	0.84446900
H	2.76513300	3.04138600	2.12522600

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1 imaginary frequency

H = -5472.460905

G = -5472.671219

E(M06-2X-DCM) = -5473.439984

C	-3.37639700	3.27773700	1.09188500
C	-3.31495800	2.37930500	2.38289500
H	-4.27809600	1.88098000	2.46547800
H	-3.26756400	3.09212700	3.22176700
C	-2.20501000	1.42190200	2.73194900
C	-2.09356900	4.11972400	0.87240300
H	-2.31630500	4.95871300	0.20216900
H	-1.78629700	4.58593400	1.81431400
N	-0.98158200	3.35208000	0.33767300
C	0.27790500	3.85409300	0.20252800
N	1.16083200	2.90240400	-0.25377300
C	2.48452100	2.98115700	-0.70493500
C	3.26976500	4.14222300	-0.75402800
C	3.03881700	1.76857100	-1.16485400
C	4.57528800	4.07442500	-1.24992700
C	4.33537600	1.72913700	-1.66057700
H	2.43556500	0.86797100	-1.15186500
C	5.12478600	2.88183000	-1.70805200
H	6.13212300	2.85099200	-2.10596900
C	4.91085200	0.44140100	-2.18000800
C	5.41718700	5.32500900	-1.23004700
F	3.98444500	-0.54466500	-2.25491500
F	5.42243400	0.59558700	-3.42556500
F	5.91899500	-0.02458000	-1.40594000
F	6.43196400	5.26341400	-2.12192400
F	4.69218500	6.42620600	-1.51568100
F	5.97498500	5.52534200	-0.01286800
S	0.62908500	5.45095300	0.61467800
C	-4.50590000	4.36189100	1.36881400
H	-4.67114300	4.88129000	0.42172000
H	-4.06466900	5.10496000	2.04767300
H	2.86070100	5.08309700	-0.41503300
C	-2.43407200	0.05411800	2.99547400
H	0.82358000	1.93848000	-0.18140300
H	-1.19277100	2.44873900	-0.07238100
H	-2.08010200	-0.47419700	1.81414600
O	0.79209100	-2.26445600	1.15813500
O	0.29025100	-1.45403000	-1.29339800

P	-0.03830200	-1.17220900	0.27469100
O	0.33861800	0.24843900	0.53424800
C	4.99120000	-2.15715200	1.05085500
C	4.26956300	-2.82117100	0.06690500
C	2.87036800	-2.91231700	0.13819700
C	2.90313700	-1.65761400	2.22823000
C	4.30584300	-1.61755400	2.13527700
C	0.24370900	-2.64494100	-2.04070900
C	1.02294700	-3.74342200	-1.67335300
C	0.72882500	-5.00020400	-2.22766600
C	-0.17036300	-5.11568100	-3.27947900
C	-0.73818500	-3.95581100	-3.79918200
C	-0.56578000	-2.69537200	-3.19657500
H	4.85703300	-1.14517200	2.94274100
H	-1.35606100	-4.01440800	-4.68892200
C	2.35403400	-3.86037100	-0.93200900
C	3.51591500	-3.75454100	-1.98693800
H	3.56793100	-4.63593400	-2.63163500
H	3.33285200	-2.88740000	-2.62783700
H	2.27590700	-6.52686400	-2.26348400
H	0.92598600	-6.91044600	-1.20354400
C	2.19764200	-2.26221100	1.16911700
H	6.07299900	-2.07721500	0.98996200
H	-0.38702800	-6.08139900	-3.72887400
C	4.79546000	-3.52081700	-1.16253500
H	5.53646800	-2.91462600	-1.69433800
H	5.28606700	-4.46766900	-0.89675500
C	1.55158300	-6.08606700	-1.56542300
C	2.25604400	-5.33077700	-0.41545400
H	1.62919600	-5.34809000	0.48368100
H	3.23404700	-5.74806800	-0.15545800
C	-1.15673000	-1.51679400	-3.90808100
C	-2.53091100	-1.53222800	-4.27177600
C	-0.30383700	-0.50098900	-4.42345200
C	-3.46467000	-2.48754700	-3.74995400
C	-3.03536400	-0.56288800	-5.21805400
C	-0.84835000	0.50857500	-5.30582100
C	-4.76665200	-2.52389700	-4.18050300
H	-3.13444500	-3.17457200	-2.98166900
C	-4.39412800	-0.65074500	-5.65894700
C	-2.18817400	0.43911000	-5.69327100
C	-5.23739000	-1.60989300	-5.16587300
H	-5.44991100	-3.25737200	-3.76082400
H	-4.74136400	0.06954800	-6.39654200

H	-2.57488500	1.17348000	-6.39736400
H	-6.26659500	-1.66832200	-5.51018300
C	2.30012200	-1.15090500	3.50114500
C	2.39917000	0.22293600	3.83112000
C	1.80126300	-2.07843100	4.45140600
C	2.86174300	1.20986300	2.90062300
C	2.01489100	0.67205200	5.15121500
C	1.40789400	-1.61253500	5.76273500
C	2.95067800	2.53295700	3.24901300
H	3.12710300	0.89733400	1.89747300
C	2.13339900	2.06054600	5.47729300
C	1.53543200	-0.25635800	6.07916900
C	2.58874600	2.96634100	4.55699400
H	3.28937800	3.26300400	2.51980300
H	1.85144100	2.37960100	6.47822400
H	1.25590300	0.08396600	7.07452400
H	2.67102200	4.01856800	4.81420900
C	1.89583700	0.54379500	-4.69584000
H	2.96106500	0.54768400	-4.48867400
C	1.10481200	-0.44439700	-4.16856200
H	1.56216800	-1.20687400	-3.55166800
C	1.34017700	1.55926600	-5.52280300
H	1.98077900	2.33979400	-5.92383200
C	0.00555500	1.53440400	-5.81959300
H	-0.43427300	2.28953400	-6.46696800
C	1.20030100	-4.34910500	5.12938100
H	1.12200700	-5.40791000	4.89793700
C	0.80101100	-3.88194700	6.41355200
H	0.41914400	-4.58551200	7.14820600
C	0.90774500	-2.55199800	6.71812200
H	0.61552000	-2.18187900	7.69812400
C	1.68666800	-3.48116900	4.18648300
H	1.99487300	-3.85993500	3.21908300
N	-1.60648600	-1.43412600	0.77144300
S	-2.60421100	-2.67948600	0.44081500
C	-2.24560000	-4.03631200	1.69280900
O	-3.97056300	-2.25438800	0.75097900
O	-2.29535600	-3.33074000	-0.83241600
F	-3.04764600	-5.06778600	1.42116600
F	-2.49491100	-3.62425600	2.94647000
F	-0.97512400	-4.43748000	1.61561600
C	-3.73279000	2.49269400	-0.18055600
C	-4.19359400	1.17148800	-0.16492800
C	-3.67036200	3.14240700	-1.42911000

C	-4.61822700	0.53261000	-1.33250900
H	-4.23513000	0.60823400	0.75564900
C	-4.09348500	2.51096600	-2.59506000
H	-3.30072900	4.16135300	-1.49703900
C	-4.58696500	1.20543700	-2.55052200
H	-4.96066300	-0.49583900	-1.27690400
H	-4.03585600	3.04135500	-3.54185300
H	-4.92453300	0.71278100	-3.45509100
C	-5.83005500	3.90658100	1.96670800
C	-6.91303400	3.58392900	1.22583200
C	-5.90506700	3.91220600	3.49207800
H	-6.80678400	4.41885700	3.85213200
H	-5.91015100	2.90522800	3.93107100
H	-5.05242400	4.44452900	3.92630800
C	-0.85697900	1.99952000	3.02793800
H	-0.07525600	1.49715300	2.44972600
H	-0.79636700	3.06868400	2.84371100
H	-0.62034400	1.81680400	4.08500300
C	-1.40176900	-0.66094500	3.87782800
H	-1.49006900	-0.31480000	4.91572000
H	-1.57637400	-1.73586100	3.86836600
H	-0.37733900	-0.49093800	3.55115700
C	-8.21683800	3.13338600	1.84963700
H	-8.99171700	3.90498300	1.73133600
H	-8.59270700	2.23982600	1.33395400
H	-8.14078200	2.89402500	2.91179200
C	-6.99083600	3.64141100	-0.28122000
H	-7.93215300	4.11843600	-0.58648200
H	-6.16940200	4.18544700	-0.74778500
H	-6.99382500	2.63218800	-0.71359100
C	-3.85997600	-0.45037100	3.26894000
H	-4.20146600	-0.06246900	4.23791000
H	-4.59494600	-0.17793200	2.51206700
H	-3.86055800	-1.53859400	3.32537800

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l imaginary frequency

H = -5472.463682

G = -5472.674820

E(M06-2X-DCM) = -5473.439349

C	-3.97339800	2.75534700	-0.63388700
C	-4.07645200	2.16834500	0.82252900
H	-4.94739400	1.51637800	0.83712800
H	-4.34535000	3.03092600	1.45480900

C	-2.95612800	1.55909300	1.62502300
C	-2.77471000	3.71541800	-0.84653600
H	-2.94533500	4.30192500	-1.75807800
H	-2.72722300	4.44973900	-0.03651200
N	-1.49226200	3.03830600	-0.93719500
C	-0.30231900	3.70388600	-0.94801600
N	0.76871300	2.83991100	-0.96859300
C	2.13812200	3.04795500	-1.18145300
C	2.74578300	4.27836900	-1.47193000
C	2.94299700	1.89168200	-1.12734500
C	4.12464100	4.33506700	-1.69403600
C	4.30964800	1.97289400	-1.36199900
H	2.48297500	0.93106000	-0.92612300
C	4.92217200	3.19673500	-1.64516700
H	5.98654600	3.25519400	-1.83926400
C	5.15845000	0.73298800	-1.33733200
C	4.75933700	5.68017600	-1.94056600
F	4.41528300	-0.39801200	-1.27342700
F	5.92614500	0.63738600	-2.45030700
F	6.00699000	0.70569100	-0.28269800
F	5.93656000	5.56837200	-2.59706600
F	3.96292300	6.48816700	-2.67078500
F	5.01694300	6.32577900	-0.77904700
S	-0.24333200	5.38775000	-0.88358600
C	-5.24193500	3.69460500	-0.78804700
H	-5.27657100	4.01647100	-1.83485400
H	-5.02849800	4.59580900	-0.20727600
H	2.14695600	5.17569100	-1.52672900
C	-3.06246600	0.28111100	2.21518700
H	0.55164700	1.88331600	-0.67471600
H	-1.50183200	2.05376000	-1.18115100
H	-2.33079900	-0.45823400	1.36279700
O	0.83305800	-1.76124200	1.85012800
O	0.83114600	-1.70665700	-0.77515000
P	0.10032400	-1.10716700	0.54832700
O	0.20656200	0.37792300	0.45185200
C	4.86998700	-0.82511900	2.53648600
C	4.51430500	-1.84968800	1.66813300
C	3.16833500	-2.20556600	1.48780500
C	2.50812600	-0.48231700	3.08233600
C	3.87018400	-0.18010800	3.25869500
C	1.13400900	-3.03183000	-1.13634900
C	1.95698400	-3.81969400	-0.32998600
C	1.98517700	-5.20821500	-0.54285900

C	1.38477200	-5.76487400	-1.66431900
C	0.78579400	-4.91460600	-2.58986800
C	0.62490400	-3.53716100	-2.35214500
H	4.13356500	0.58512400	3.98257900
H	0.40195200	-5.31933900	-3.52045200
C	3.06980700	-3.47640600	0.65935900
C	4.42935100	-3.40791500	-0.12874500
H	4.76348200	-4.39545400	-0.45781700
H	4.28998300	-2.79273800	-1.02162700
H	3.69675700	-6.34664000	0.16651100
H	2.19743600	-6.72235900	1.00542600
C	2.17866200	-1.46875200	2.13241600
H	5.91101100	-0.54335400	2.66831900
H	1.42244100	-6.83571300	-1.84710200
C	5.42001700	-2.71274100	0.82401900
H	6.17220100	-2.12013500	0.29249400
H	5.96323800	-3.43831000	1.44558000
C	2.76833700	-5.90388400	0.55150700
C	3.05473700	-4.75905800	1.54988000
H	2.23476800	-4.67820100	2.27307900
H	3.98749200	-4.89067900	2.10753300
C	0.02447100	-2.71905300	-3.45345600
C	-1.22965500	-3.09516600	-4.00594600
C	0.80109000	-1.71134800	-4.08961000
C	-2.09051600	-4.06714300	-3.39628800
C	-1.67830800	-2.49652400	-5.24271600
C	0.29900500	-1.07222800	-5.28656200
C	-3.26333400	-4.45723100	-3.99127100
H	-1.81503400	-4.47829800	-2.43390100
C	-2.89613500	-2.95000700	-5.84222000
C	-0.91353700	-1.49214700	-5.83770400
C	-3.66629700	-3.90973100	-5.24259100
H	-3.89601500	-5.19104800	-3.49927700
H	-3.19558500	-2.50885600	-6.79058600
H	-1.26095000	-1.03625600	-6.76285500
H	-4.58818600	-4.24720300	-5.70884200
C	1.54107800	0.19939800	3.99920900
C	1.36368500	1.60250300	3.91991900
C	0.94982600	-0.53550500	5.05868200
C	1.90133400	2.39038700	2.85020700
C	0.60389100	2.28716300	4.94260500
C	0.17975500	0.16084900	6.06541500
C	1.71632000	3.74803200	2.80104800
H	2.44591900	1.89125900	2.05733700

C	0.44550400	3.70720800	4.86022300
C	0.03874100	1.54990400	5.98665000
C	0.98542000	4.41959400	3.82306400
H	2.11798400	4.31972900	1.96965700
H	-0.11767600	4.20816800	5.64448800
H	-0.52488600	2.06981100	6.75912900
H	0.85476900	5.49662500	3.76787100
C	2.82953500	-0.35295100	-4.29296500
H	3.81841400	-0.08915700	-3.93164200
C	2.10483800	-1.31924800	-3.64400400
H	2.53600900	-1.80470000	-2.77810700
C	2.30607400	0.30195600	-5.44244800
H	2.89063300	1.07206200	-5.93809900
C	1.07649600	-0.05471600	-5.92343000
H	0.66789200	0.42058800	-6.81216800
C	0.51089500	-2.63083400	6.23934000
H	0.63745900	-3.70707400	6.31963500
C	-0.25837700	-1.94143000	7.21900600
H	-0.71410700	-2.49607200	8.03463300
C	-0.41273300	-0.58435500	7.13274900
H	-0.98954700	-0.04285100	7.87898300
C	1.09697800	-1.95283300	5.20220300
H	1.68740900	-2.49608600	4.47385100
N	-1.49350800	-1.53853000	0.78144300
S	-2.18705100	-3.00965700	0.65596400
C	-2.03650100	-3.85572300	2.32996300
O	-3.62586700	-2.81247200	0.47129000
O	-1.43695900	-3.91295700	-0.21732100
F	-2.54915200	-5.08225400	2.21352900
F	-2.72323300	-3.19872900	3.27898100
F	-0.76039400	-3.94715000	2.70739300
C	-3.96892000	1.67324600	-1.72736100
C	-3.95240700	0.30017400	-1.45285500
C	-4.01081800	2.06482700	-3.07919500
C	-4.03507300	-0.64870400	-2.47615300
H	-3.88717700	-0.06258000	-0.43653500
C	-4.09278100	1.12417700	-4.10159100
H	-3.99236400	3.11821900	-3.34369800
C	-4.12400100	-0.23966100	-3.80389800
H	-4.03057200	-1.70377700	-2.22106100
H	-4.13601600	1.45974400	-5.13456200
H	-4.20076600	-0.97644700	-4.59556000
C	-6.60782700	3.13539000	-0.41804500
C	-7.27868400	3.50932200	0.69625700

C	-7.18004500	2.17023100	-1.44029900
H	-8.25741100	2.02965100	-1.34210400
H	-6.98930000	2.53793100	-2.45536400
H	-6.70709000	1.18215900	-1.38519500
C	-1.81056500	2.44182800	2.00764800
H	-0.85231300	1.96945700	1.76960900
H	-1.84482800	3.42110700	1.53825700
H	-1.82086100	2.58175300	3.09717600
C	-2.22363800	0.03598700	3.47863700
H	-2.63037900	0.61539700	4.31764100
H	-2.25363600	-1.01679100	3.75488600
H	-1.17865900	0.31434300	3.35121800
C	-8.64251000	2.97379100	1.08158300
H	-8.62649900	2.61536900	2.12007800
H	-9.39673900	3.77301900	1.04616400
H	-8.99525900	2.15080600	0.45988200
C	-6.78528100	4.51092400	1.72061100
H	-6.60724900	4.02085200	2.68883600
H	-5.87106300	5.03885200	1.44432000
H	-7.55765700	5.27036300	1.90425200
C	-4.43213600	-0.41407400	2.27962600
H	-5.10009500	0.14705000	2.94636100
H	-4.92432800	-0.52591700	1.31308600
H	-4.31762400	-1.41735600	2.68861600

TS-1-1-7SR-2

l imaginary frequency

H = -5472.460479

G = -5472.671212

E(M06-2X-DCM) = -5473.439042

C	-3.87144100	1.45374200	2.48032500
C	-3.06848000	0.64635300	3.58116700
H	-3.68232900	-0.20925000	3.85856700
H	-3.06264100	1.30870600	4.46245800
C	-1.62302700	0.23270200	3.49519200
C	-3.15660800	2.75109000	2.04183600
H	-3.86479800	3.41441200	1.53936800
H	-2.81450200	3.30853600	2.92079600
N	-2.02442200	2.51221900	1.15985100
C	-1.18133600	3.49927800	0.74606100
N	-0.16473100	3.00800300	-0.03968900
C	0.82493800	3.63516200	-0.80748300
C	1.06642900	5.01506500	-0.87322400
C	1.62469000	2.76979200	-1.58276800

C	2. 08771900	5. 50051100	-1. 69590700
C	2. 62809900	3. 27728500	-2. 39733500
H	1. 43484500	1. 70286900	-1. 55690700
C	2. 87649700	4. 65145700	-2. 46442300
H	3. 65278700	5. 04622800	-3. 10907100
C	3. 45522500	2. 35532500	-3. 24882600
C	2. 36644000	6. 98220500	-1. 69487300
F	3. 00961000	1. 07635400	-3. 20903200
F	3. 43959400	2. 73662000	-4. 54936200
F	4. 75529300	2. 33111500	-2. 87185500
F	3. 02410600	7. 37242300	-2. 81020300
F	1. 23260300	7. 70889400	-1. 61698500
F	3. 13581300	7. 33870900	-0. 63932100
S	-1. 41099600	5. 10012700	1. 22536200
C	-5. 18533600	1. 86804900	3. 28074500
H	-4. 84587400	2. 45877500	4. 14369200
H	-5. 59208500	0. 94070800	3. 69245100
H	0. 45771200	5. 69538300	-0. 29502200
C	-1. 20503000	-1. 11038000	3. 62034900
H	-0. 05860000	1. 99003000	-0. 01362100
H	-1. 95650900	1. 59918600	0. 72310700
H	-1. 05553200	-1. 43086700	2. 33087900
O	1. 94034000	-1. 86657100	0. 67392900
O	0. 43884900	-1. 29765800	-1. 40906800
P	0. 52190200	-1. 20420000	0. 21306900
O	0. 37368300	0. 24011100	0. 56015500
C	5. 51069800	-0. 02336100	-0. 55453200
C	4. 84304700	-0. 91155300	-1. 38839200
C	3. 68575100	-1. 57616400	-0. 95270200
C	3. 86293800	-0. 45500500	1. 20476900
C	5. 03655500	0. 16539700	0. 74028200
C	0. 63492900	-2. 38967900	-2. 27417000
C	1. 85304400	-3. 07163000	-2. 28983200
C	1. 91936200	-4. 32920400	-2. 91216600
C	0. 86231000	-4. 79180400	-3. 68466900
C	-0. 24227900	-3. 96394900	-3. 86375400
C	-0. 40107300	-2. 75397800	-3. 16181600
H	5. 57778400	0. 81062700	1. 42563100
H	-1. 02736400	-4. 26025200	-4. 55121600
C	3. 28110900	-2. 63694000	-1. 96325700
C	3. 92661500	-2. 04356400	-3. 26918800
H	4. 12025100	-2. 81484100	-4. 01943800
H	3. 23290900	-1. 32181700	-3. 70975800
H	3. 84815200	-5. 07622600	-3. 58071000

H	3. 15026200	-6. 00033000	-2. 25711100
C	3. 16264400	-1. 28043300	0. 30294800
H	6. 40005200	0. 49939400	-0. 89536500
H	0. 91405400	-5. 75389600	-4. 18786800
C	5. 19771500	-1. 31169800	-2. 79968700
H	5. 44148000	-0. 44493300	-3. 42302600
H	6. 07519400	-1. 97332800	-2. 81199000
C	3. 26050900	-4. 98561900	-2. 65728100
C	3. 92854700	-4. 02287300	-1. 64937000
H	3. 66583000	-4. 31139100	-0. 62494600
H	5. 02023700	-4. 00071300	-1. 72649700
C	-1. 59103400	-1. 91603300	-3. 51741500
C	-2. 88886400	-2. 49595300	-3. 49806500
C	-1. 40351600	-0. 63051400	-4. 09806100
C	-3. 16868200	-3. 75934800	-2. 87980000
C	-3. 99191400	-1. 81204100	-4. 13439600
C	-2. 53842500	0. 07328800	-4. 65580000
C	-4. 41452800	-4. 32928400	-2. 94946500
H	-2. 38188500	-4. 25553700	-2. 32647200
C	-5. 27002600	-2. 45207400	-4. 20549400
C	-3. 79181300	-0. 54210600	-4. 67741900
C	-5. 47769200	-3. 68205200	-3. 64134800
H	-4. 59449800	-5. 28564600	-2. 46579900
H	-6. 07596700	-1. 93206000	-4. 71877700
H	-4. 62747900	-0. 02595200	-5. 14631900
H	-6. 45199800	-4. 15955100	-3. 70427600
C	3. 53119000	-0. 26656000	2. 65216400
C	3. 18634700	1. 01946100	3. 13548600
C	3. 74570700	-1. 33549700	3. 55970100
C	2. 92299700	2. 12706900	2. 26506000
C	3. 08116800	1. 24487000	4. 56028800
C	3. 62319000	-1. 09838200	4. 98104500
C	2. 59635800	3. 36281400	2. 76123200
H	2. 96772900	1. 97059400	1. 19364000
C	2. 74702000	2. 55246700	5. 03651900
C	3. 30628500	0. 18359400	5. 44116400
C	2. 51303100	3. 58331800	4. 16621700
H	2. 38819800	4. 18190100	2. 07910500
H	2. 68362300	2. 70771600	6. 11124200
H	3. 23522500	0. 35922400	6. 51298000
H	2. 25710900	4. 57109500	4. 53897800
C	0. 01598800	1. 23837400	-4. 80317200
H	1. 00251700	1. 68203500	-4. 89024700
C	-0. 12487800	0. 00324000	-4. 22446100

H	0.75760300	-0.50857300	-3.86343900
C	-1.11435900	1.94226900	-5.30383000
H	-0.98478300	2.92417100	-5.75048800
C	-2.35360600	1.36848100	-5.23352200
H	-3.22702600	1.88118600	-5.62981200
C	4.30715000	-3.66504700	4.04442500
H	4.57764500	-4.65755100	3.69440100
C	4.17049500	-3.42870200	5.44164100
H	4.33392300	-4.24126000	6.14419200
C	3.84235700	-2.17881900	5.89218000
H	3.74379800	-1.98086900	6.95702300
C	4.10759000	-2.65567600	3.13875200
H	4.22750600	-2.85530000	2.08045400
N	-0.58520000	-2.10055900	1.07409000
S	-1.06533000	-3.64293800	0.86091000
C	0.16434300	-4.74217000	1.76452400
O	-2.31943300	-3.82812600	1.59331600
O	-0.93691600	-4.09140100	-0.52590100
F	-0.21133300	-6.01060700	1.58854000
F	0.17603800	-4.48258000	3.08233500
F	1.39840000	-4.58044200	1.28257100
C	-4.25593200	0.59873500	1.26383100
C	-4.17130300	-0.80003400	1.25894600
C	-4.79524000	1.21769100	0.11965000
C	-4.64122200	-1.55817600	0.18552300
H	-3.73320400	-1.33307100	2.09019700
C	-5.26881000	0.46471400	-0.95242500
H	-4.86066300	2.29807100	0.06202600
C	-5.21036500	-0.92945500	-0.91838900
H	-4.54284300	-2.63856200	0.21809800
H	-5.68025700	0.97272000	-1.82065900
H	-5.58247000	-1.51697200	-1.74984600
C	-6.28262800	2.65419700	2.58697800
C	-7.39082000	2.07415200	2.07517600
C	-6.10781900	4.16998100	2.57790400
H	-6.98149700	4.68250600	2.99689100
H	-5.24484700	4.47541300	3.17651600
H	-5.95342000	4.57753800	1.57026300
C	-0.59162900	1.31639900	3.50100700
H	0.11503000	1.19614500	2.67402700
H	-1.01764100	2.31515600	3.45576900
H	0.00000600	1.23245000	4.42295400
C	0.23964100	-1.34214600	4.08269300
H	0.34156400	-1.08160700	5.14409200

H	0.50872300	-2.39132900	3.96909400
H	0.96198000	-0.75400600	3.51944700
C	-8.49498000	2.87231500	1.41811700
H	-8.67155400	2.50599300	0.39720300
H	-9.44294500	2.74028900	1.95906900
H	-8.29000700	3.94205100	1.35493300
C	-7.67919900	0.59149900	2.07001700
H	-7.68096600	0.20782800	1.04110700
H	-6.96162400	-0.00890600	2.63034400
H	-8.67998700	0.39856300	2.48083800
C	-2.16003700	-2.16584700	4.20117700
H	-2.31382700	-1.96608000	5.26987400
H	-3.13460200	-2.21776500	3.71692800
H	-1.71407300	-3.15548000	4.10601800

TS-1-1-7RS

1 imaginary frequency

H = -5472.469061

G = -5472.678016

E(M06-2X-DCM) = -5473.445212

C	3.40491000	2.43215900	2.06320300
C	2.35494900	2.13201300	3.21996400
H	2.95008100	1.75508400	4.05927100
H	1.95702400	3.11007000	3.51492500
C	1.13337900	1.24183900	3.09759700
C	2.76017900	3.11869200	0.82559900
H	3.48070200	3.08370600	-0.00058100
H	2.61012600	4.17234600	1.05643000
N	1.46489800	2.63928200	0.37326900
C	0.47083500	3.47130100	-0.06218000
N	-0.59116000	2.77228900	-0.58581900
C	-1.83036500	3.20829500	-1.08174600
C	-2.51209100	4.35004100	-0.63178100
C	-2.44424100	2.38425700	-2.03721200
C	-3.76925200	4.65317000	-1.15163200
C	-3.70362900	2.70284800	-2.54220600
H	-1.93191500	1.49295300	-2.38612100
C	-4.37727900	3.84474100	-2.11322200
H	-5.34953900	4.09970300	-2.51701500
C	-4.36790200	1.75419600	-3.49944000
C	-4.53690000	5.82455300	-0.59693900
F	-3.48382400	1.19624500	-4.36026900
F	-5.32866400	2.34935300	-4.23257800
F	-4.96159600	0.72086900	-2.83897100

F	-3.73089800	6.77103900	-0.08068100
F	-5.37573700	5.43342300	0.40005700
F	-5.30888500	6.40947500	-1.53916400
S	0.54396200	5.15660200	0.04373100
H	-2.05894200	4.99061300	0.11032500
C	1.10481000	-0.11874000	3.46579900
H	-0.45831600	1.75876800	-0.64137900
H	1.35314500	1.64956300	0.16062900
H	0.94965500	-0.81377100	2.31663000
O	-1.74125600	-1.38046000	0.03040200
O	0.35370000	-2.31308400	-1.24084600
P	-0.11411500	-1.31524500	-0.04475600
O	0.23569000	0.11845700	-0.27953000
C	-3.93211700	-4.94661900	0.39505100
C	-3.28081500	-4.63290500	-0.79106600
C	-2.65132300	-3.38971200	-0.95288700
C	-3.26032200	-2.77988300	1.32811400
C	-3.96415000	-3.99694000	1.41108100
C	-0.00261400	-1.97071100	-2.56299100
C	-1.28986700	-2.26616900	-3.01182400
C	-1.70939700	-1.78528600	-4.26396500
C	-0.83012800	-1.10102800	-5.09381000
C	0.48744600	-0.93266500	-4.67926300
C	0.93717200	-1.35668700	-3.41499300
H	-4.53678300	-4.19378700	2.31146000
H	1.20391300	-0.45353700	-5.33932400
C	-2.36648600	-3.17431800	-2.43333100
C	-2.15988600	-4.65385600	-2.89773600
H	-2.30195600	-4.77663300	-3.97584500
H	-1.13552200	-4.95826100	-2.65480700
H	-3.72390700	-1.27888600	-4.90800400
H	-3.24462000	-2.93979900	-5.25838900
C	-2.53567700	-2.53489800	0.14143700
H	-4.44112600	-5.89894800	0.51899600
H	-1.15374900	-0.72599500	-6.06106300
C	-3.16185300	-5.46522100	-2.04874900
H	-4.13148100	-5.56677300	-2.55543700
H	-2.80894800	-6.48147400	-1.83935400
C	-3.15774200	-2.13074500	-4.51981500
C	-3.64016400	-2.57803900	-3.12745700
H	-4.46808800	-3.29209000	-3.15871400
H	-3.97728400	-1.70160100	-2.56355800
C	2.40481600	-1.20793900	-3.15447600
C	3.23611200	-2.35701200	-3.18339800

C	2. 98152500	0. 08556700	-3. 11183600
C	2. 72170400	-3. 69202300	-3. 24785400
C	4. 67383700	-2. 19560300	-3. 19222700
C	4. 41969300	0. 23138400	-3. 13845000
C	3. 55569700	-4. 77872700	-3. 28271800
H	1. 64869900	-3. 84163600	-3. 26793900
C	5. 50845500	-3. 35686400	-3. 22723500
C	5. 22393200	-0. 91016500	-3. 18584400
C	4. 96965700	-4. 61403400	-3. 26690200
H	3. 13488500	-5. 77960700	-3. 32451200
H	6. 58656000	-3. 21423500	-3. 22619100
H	6. 30572700	-0. 79623400	-3. 21100000
H	5. 61431000	-5. 48824500	-3. 29336500
C	-3. 41871400	-1. 81175400	2. 45650100
C	-3. 98864400	-0. 53176500	2. 21989700
C	-3. 14144800	-2. 22832500	3. 78651800
C	-4. 38198100	-0. 07468500	0. 92091200
C	-4. 23842800	0. 35784800	3. 33330700
C	-3. 46395800	-1. 35324100	4. 89213800
C	-4. 90529400	1. 17640200	0. 72659400
H	-4. 27592400	-0. 73910000	0. 07256400
C	-4. 76540900	1. 66545800	3. 08493100
C	-3. 98588500	-0. 08277600	4. 63512800
C	-5. 07859300	2. 07483400	1. 81731000
H	-5. 19365300	1. 48140900	-0. 27387100
H	-4. 91818100	2. 32622000	3. 93525000
H	-4. 20749000	0. 57856100	5. 47072300
H	-5. 45889100	3. 07530400	1. 63293900
C	2. 77870600	2. 52229000	-3. 02666600
H	2. 15832500	3. 41227100	-2. 96790700
C	2. 19448600	1. 28161500	-3. 04758500
H	1. 11555100	1. 19183900	-3. 00181300
C	4. 19657300	2. 65831300	-3. 06875100
H	4. 64109400	3. 64954300	-3. 05637700
C	4. 98939000	1. 54312100	-3. 11834900
H	6. 07279200	1. 63284100	-3. 14291000
C	-2. 29016400	-3. 86147900	5. 39734100
H	-1. 80389800	-4. 81172100	5. 59870400
C	-2. 65925500	-3. 01700400	6. 48181600
H	-2. 47747900	-3. 33977400	7. 50339600
C	-3. 21972200	-1. 79388400	6. 23087700
H	-3. 48717800	-1. 12676400	7. 04723800
C	-2. 51992200	-3. 48151200	4. 10009700
H	-2. 19947900	-4. 12785200	3. 29220100

N	0.61056000	-1.86467100	1.34020900
S	0.78036800	-3.44816800	1.75125600
C	2.53507800	-3.85145500	1.23032200
O	-0.08263000	-4.32287300	0.95555500
O	0.81017000	-3.56890700	3.20993200
F	2.71799300	-5.16887400	1.35154900
F	2.75741300	-3.49071100	-0.03401700
F	3.39707800	-3.21596400	2.02961800
C	4.18979100	1.14815500	1.74035200
C	5.15260700	0.65307100	2.64044400
C	3.96461700	0.40720700	0.57378200
C	5.87339600	-0.50955500	2.37703100
H	5.34954900	1.17376500	3.57217100
C	4.66822900	-0.77242300	0.31546900
H	3.24179700	0.73811200	-0.16332500
C	5.63306400	-1.23120000	1.20788400
H	6.61575300	-0.85364100	3.09257900
H	4.45204600	-1.33243100	-0.58578000
H	6.18104000	-2.14627500	1.00166900
C	4.35442200	3.54342500	2.68015300
H	3.69737200	4.26919100	3.16137900
H	4.94209400	3.09352800	3.48835200
C	5.30166600	4.26545200	1.73017500
C	5.14410000	5.56883600	1.40221000
C	-0.21510900	-0.60659900	4.09873100
H	-1.08755500	-0.38450500	3.48617500
H	-0.17489600	-1.68490200	4.24526100
H	-0.35204000	-0.12708500	5.07700700
C	6.04968500	6.31071900	0.44014900
H	5.44117300	6.84417100	-0.30253600
H	6.63224800	7.07965800	0.96778500
H	6.74730100	5.67540800	-0.10657900
C	6.45734100	3.42437600	1.22216600
H	7.26410800	4.02276600	0.79633100
H	6.88798700	2.83272800	2.03862900
H	6.13938800	2.70110500	0.46035300
C	-0.16755100	1.95019700	2.84413800
H	-0.02544400	2.97236400	2.49713900
H	-0.79745800	1.41274400	2.12862400
H	-0.73563100	1.98045400	3.78612600
C	2.33564100	-0.75720200	4.11348400
H	3.24736300	-0.59550800	3.54171500
H	2.48238500	-0.35101300	5.12480000
H	2.18285900	-1.83317900	4.21041800

C	4. 04564200	6. 47796700	1. 91640300
H	3. 27568700	6. 63415200	1. 14849200
H	3. 53798700	6. 11861900	2. 81354100
H	4. 46209800	7. 46620400	2. 15199600

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1 imaginary frequency

H = -5472. 466558

G = -5472. 675602

E(M06-2X-DCM) = -5473. 442696

C	3. 58553600	2. 66774500	1. 22375900
C	2. 63271400	2. 53333200	2. 49278000
H	3. 30284600	2. 26318000	3. 31652300
H	2. 26838700	3. 54980900	2. 68489400
C	1. 41279200	1. 64233500	2. 62705700
C	2. 80287700	3. 09979800	-0. 05913500
H	3. 37218700	2. 79334700	-0. 94138700
H	2. 73698000	4. 18646300	-0. 07929000
N	1. 43220700	2. 64116100	-0. 20702100
C	0. 39975800	3. 46813100	-0. 56295900
N	-0. 73252600	2. 75744200	-0. 88024500
C	-2. 02195400	3. 17379400	-1. 24724200
C	-2. 62184500	4. 37733200	-0. 84506100
C	-2. 76928100	2. 26585500	-2. 01350500
C	-3. 93431500	4. 65411000	-1. 22505300
C	-4. 08009800	2. 56079900	-2. 38180300
H	-2. 31968500	1. 32711200	-2. 32213000
C	-4. 67610000	3. 76131800	-1. 99978200
H	-5. 69053400	3. 99659600	-2. 29789600
C	-4. 87727100	1. 52941300	-3. 12927100
C	-4. 60573800	5. 90019200	-0. 70929800
F	-4. 12121700	0. 85313100	-4. 02664400
F	-5. 91788800	2. 06519300	-3. 79597200
F	-5. 39247100	0. 59426800	-2. 28288700
F	-3. 72658900	6. 87935000	-0. 42587900
F	-5. 29689800	5. 64659100	0. 43441900
F	-5. 49903300	6. 39206600	-1. 59584200
S	0. 51381600	5. 15348900	-0. 58522300
H	-2. 06421800	5. 08477900	-0. 24914300
C	1. 45190500	0. 33141900	3. 14466900
H	-0. 62016000	1. 74009200	-0. 86837400
H	1. 27231100	1. 64333700	-0. 33742400
H	1. 12823000	-0. 50372400	2. 12352800
O	-1. 83488100	-1. 28223200	0. 29628000

O	0.06836400	-2.42351100	-1.09609000
P	-0.23154000	-1.26744800	0.00648300
O	0.09483600	0.11400100	-0.45995300
C	-4.02084200	-4.71917500	1.32510400
C	-3.52433800	-4.55466100	0.03830000
C	-2.89536500	-3.35828400	-0.33857900
C	-3.18882100	-2.49120700	1.92270200
C	-3.89843900	-3.66835900	2.22834200
C	-0.43251300	-2.22612000	-2.40032600
C	-1.76912200	-2.52419300	-2.66083800
C	-2.32082200	-2.17529800	-3.90531700
C	-1.52674800	-1.62990400	-4.90665200
C	-0.16598500	-1.46080300	-4.66657900
C	0.41527000	-1.74486200	-3.41736100
H	-4.34839300	-3.75096300	3.21227800
H	0.47944500	-1.08702600	-5.45550800
C	-2.79125100	-3.31727000	-1.85839100
C	-2.67934100	-4.84581500	-2.17327700
H	-2.95644700	-5.08026500	-3.20563600
H	-1.64026100	-5.15986200	-2.02259400
H	-4.38346600	-1.65801600	-4.36149100
H	-4.00023900	-3.36685300	-4.57105600
C	-2.62400900	-2.39571600	0.63250100
H	-4.52797300	-5.63549200	1.61590100
H	-1.95147200	-1.36039100	-5.87001200
C	-3.58699500	-5.52107800	-1.12372200
H	-4.61518100	-5.63680200	-1.49348500
H	-3.23787700	-6.52257800	-0.84758200
C	-3.79936800	-2.48512100	-3.94682400
C	-4.12268000	-2.75220600	-2.46412000
H	-4.96696700	-3.43162500	-2.31591800
H	-4.36730400	-1.80524000	-1.97107800
C	1.90161000	-1.59763500	-3.31667200
C	2.71564900	-2.75777800	-3.26739400
C	2.49274800	-0.32028800	-3.47839400
C	2.18223000	-4.08132800	-3.14709000
C	4.15119200	-2.62588600	-3.38511200
C	3.92688800	-0.20706600	-3.62129500
C	2.99926700	-5.18067100	-3.10856200
H	1.10820300	-4.21148700	-3.08512500
C	4.96847900	-3.79884100	-3.33475800
C	4.71457600	-1.35977000	-3.57016300
C	4.41336900	-5.04187600	-3.19620500
H	2.56479600	-6.17180900	-3.01118300

H	6.04609700	-3.67759800	-3.41661300
H	5.79352200	-1.27000800	-3.67813700
H	5.04473800	-5.92541300	-3.16065400
C	-3.17396100	-1.40737000	2.95307700
C	-3.75744100	-0.14446600	2.66473000
C	-2.71650900	-1.69256400	4.26777300
C	-4.32353700	0.18703900	1.39170300
C	-3.84010100	0.85987900	3.70305700
C	-2.87103300	-0.70124700	5.30972000
C	-4.85822900	1.42359900	1.14283400
H	-4.34169700	-0.56220800	0.61011100
C	-4.38462000	2.14744600	3.39503300
C	-3.41158200	0.54854200	4.99614300
C	-4.86919300	2.43233100	2.14742500
H	-5.28152800	1.63187700	0.16597600
H	-4.41012600	2.89510900	4.18454200
H	-3.50728600	1.29696800	5.78061100
H	-5.26233100	3.41752200	1.91399700
C	2.32097400	2.10909200	-3.71218800
H	1.71497300	3.01060300	-3.73397900
C	1.72497000	0.88955000	-3.51743400
H	0.65166600	0.82886400	-3.38161700
C	3.73316100	2.21025800	-3.87556600
H	4.18665400	3.18422700	-4.03727000
C	4.50971800	1.08370400	-3.82203400
H	5.58926700	1.14759700	-3.93538200
C	-1.66634200	-3.17437200	5.90685100
H	-1.16753900	-4.11138200	6.13732100
C	-1.86876600	-2.21393300	6.93735100
H	-1.54809900	-2.43509100	7.95180100
C	-2.44535500	-1.00879300	6.64014100
H	-2.58750200	-0.25507500	7.41131900
C	-2.07231600	-2.92326400	4.62154900
H	-1.87720900	-3.65717200	3.84916600
N	0.66565100	-1.65127300	1.34668800
S	0.88300800	-3.17590400	1.92792400
C	2.55018100	-3.67970500	1.23296100
O	-0.08582400	-4.12098300	1.37003600
O	1.11112600	-3.11720700	3.37238900
F	2.73133000	-4.98011100	1.47590700
F	2.60921400	-3.46441000	-0.08186000
F	3.51759800	-2.98352300	1.83709300
C	4.39297200	1.37645600	1.03438800
C	5.51411600	1.11452200	1.84200200

C	4.02941200	0.39958500	0.09782700
C	6.24434600	-0.06560200	1.71378400
H	5.82243300	1.83241600	2.59257800
C	4.75075800	-0.79040300	-0.02588600
H	3.17353700	0.54540500	-0.55266300
C	5.86462600	-1.02656500	0.77665800
H	7.10789400	-0.23363500	2.35231100
H	4.42935600	-1.53429100	-0.74551800
H	6.42426800	-1.95286700	0.67981500
C	4.53117100	3.88050100	1.62949200
H	3.90940300	4.78387100	1.55005500
H	4.75305800	3.77627800	2.69143100
C	5.82710400	4.11709000	0.86436000
C	7.02350400	4.24693600	1.48221900
C	0.24636800	-0.06569700	4.02377600
H	-0.71042300	0.08923700	3.52748200
H	0.31760000	-1.11860000	4.29226200
H	0.25347800	0.53024100	4.94613900
C	8.32941100	4.49268600	0.75298000
H	8.70424800	5.50752000	0.95022300
H	9.09904800	3.80369600	1.12654800
H	8.27476600	4.35864700	-0.32754000
C	5.66834800	4.28697700	-0.63312800
H	6.53524100	4.75172600	-1.10393800
H	5.49699700	3.32607000	-1.13588900
H	4.80448700	4.92316400	-0.85928800
C	0.08285800	2.32967700	2.49675000
H	0.16245400	3.30496200	2.01910900
H	-0.64663500	1.72071300	1.95397200
H	-0.33359500	2.47378000	3.50513600
C	2.77255600	-0.23885400	3.66722200
H	3.58784500	-0.14783700	2.95221600
H	3.06547800	0.27753400	4.59315800
H	2.64732300	-1.29568300	3.90791200
C	7.25637200	4.17579800	2.97772200
H	7.83617600	5.04969900	3.30503600
H	6.35173700	4.14762300	3.58721400
H	7.86285900	3.29525500	3.23490700

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l imaginary frequency

H = -5472.467561

G = -5472.676396

E(M06-2X-DCM) = -5473.448685

C	3. 50993600	2. 37151000	1. 49820300
C	3. 07636600	1. 42945300	2. 70002900
H	3. 84125500	0. 66363500	2. 78837100
H	3. 17842500	2. 05087700	3. 60913600
C	1. 73426300	0. 80331500	2. 96777600
C	2. 43406200	3. 39394700	1. 06364600
H	2. 88377400	4. 06996400	0. 32950100
H	2. 13876500	4. 02616000	1. 90894800
N	1. 23867600	2. 82147300	0. 47024600
C	0. 16119100	3. 58414000	0. 14785100
N	-0. 88250300	2. 83222900	-0. 34768900
C	-2. 16836400	3. 21168100	-0. 76123500
C	-2. 86558600	4. 32240900	-0. 25847900
C	-2. 80860500	2. 37320500	-1. 68701800
C	-4. 16118000	4. 58379500	-0. 69975500
C	-4. 10719400	2. 64997400	-2. 11188800
H	-2. 28853500	1. 50245800	-2. 07465500
C	-4. 79568600	3. 76249000	-1. 63230800
H	-5. 79891500	3. 98415900	-1. 97505100
C	-4. 79685400	1. 68611500	-3. 03485300
C	-4. 93455500	5. 72119400	-0. 08560000
F	-3. 95131900	1. 16614100	-3. 95540500
F	-5. 82245500	2. 25268900	-3. 70023300
F	-5. 31253500	0. 62806800	-2. 34792200
F	-5. 80132800	6. 27100300	-0. 96466600
F	-4. 13364900	6. 70251700	0. 36954200
F	-5. 67668400	5. 29491600	0. 97192000
S	0. 16333400	5. 26046200	0. 34843700
C	3. 90331100	1. 55129000	0. 20365000
H	3. 98589200	2. 29341700	-0. 59407600
H	3. 04284200	0. 92793400	-0. 06721200
H	-2. 39261300	4. 97250400	0. 46265400
C	1. 62113100	-0. 55541800	3. 34558100
H	-0. 68645400	1. 83292500	-0. 44485300
H	1. 20133600	1. 82879400	0. 25323400
H	1. 24453700	-1. 08415600	2. 21174100
O	-1. 76463400	-1. 35201200	0. 13406800
O	0. 20151000	-2. 12604500	-1. 39999000
P	-0. 14647700	-1. 28363400	-0. 05673400
O	0. 20469400	0. 17008700	-0. 11234900
C	-3. 80666400	-4. 98948200	0. 61613800
C	-3. 28225500	-4. 63108300	-0. 61884200
C	-2. 72113800	-3. 35990300	-0. 81534600
C	-3. 11532200	-2. 82260300	1. 53100600

C	-3.77261600	-4.06161000	1.65293400
C	-0.33322400	-1.74008400	-2.64375700
C	-1.63126800	-2.12923400	-2.97476100
C	-2.20342800	-1.65507800	-4.16818700
C	-1.46630500	-0.88110600	-5.05555700
C	-0.13879800	-0.59495500	-4.75354400
C	0.45951800	-1.00617400	-3.54861400
H	-4.24803300	-4.29646000	2.59967700
H	0.46562600	-0.02857300	-5.45522500
C	-2.58529500	-3.11609800	-2.31335600
C	-2.33953500	-4.57742300	-2.81151200
H	-2.56251400	-4.69936700	-3.87599200
H	-1.28510300	-4.82975200	-2.65336600
H	-4.29923800	-1.29559500	-4.62167300
H	-3.73361200	-2.91465400	-5.03523500
C	-2.52335300	-2.52682200	0.28332500
H	-4.26473800	-5.96343200	0.76785300
H	-1.91064200	-0.51687800	-5.97795600
C	-3.22841500	-5.44509100	-1.89339300
H	-4.22953400	-5.59286000	-2.32116700
H	-2.80811400	-6.44291900	-1.72416000
C	-3.63908400	-2.10560200	-4.29750700
C	-3.95577700	-2.59574800	-2.87350000
H	-4.73685500	-3.36021200	-2.83584700
H	-4.28992600	-1.74741700	-2.26693500
C	1.91230800	-0.69178100	-3.37720700
C	2.87179300	-1.73127100	-3.46433900
C	2.33078900	0.66146100	-3.33428000
C	2.51638200	-3.11384500	-3.57725000
C	4.27926800	-1.40042000	-3.49203500
C	3.73811900	0.97799000	-3.41808800
C	3.47117200	-4.09275200	-3.66516100
H	1.46783700	-3.38737000	-3.59222800
C	5.24416800	-2.45350000	-3.57357500
C	4.67199900	-0.05917100	-3.48176000
C	4.85616200	-3.76352800	-3.65336700
H	3.17004800	-5.13371200	-3.74541300
H	6.29795400	-2.18468500	-3.58336000
H	5.73101400	0.18341300	-3.53728100
H	5.59859200	-4.55417100	-3.71948600
C	-3.17380300	-1.88167800	2.69174300
C	-3.79837100	-0.61365100	2.54501000
C	-2.74073500	-2.31274200	3.97450900
C	-4.35828500	-0.15320200	1.31021200

C	-3.93558800	0.25490600	3.69365000
C	-2.94444200	-1.45692500	5.12315600
C	-4.94351800	1.08069700	1.20211200
H	-4.33345300	-0.80245800	0.44392600
C	-4.52903500	1.54730500	3.53240200
C	-3.51504900	-0.19354300	4.94856200
C	-5.01138300	1.95943500	2.32002200
H	-5.36194100	1.38800700	0.24949300
H	-4.59580800	2.19303500	4.40502400
H	-3.64908200	0.45236300	5.81431100
H	-5.44605600	2.94741400	2.19994800
C	1.84246700	3.05762500	-3.23182200
H	1.12417500	3.86652600	-3.13366100
C	1.41239900	1.75587000	-3.22164900
H	0.35499100	1.54031800	-3.12288800
C	3.22790000	3.36267200	-3.36100300
H	3.54931100	4.40031800	-3.38514000
C	4.14505700	2.34929600	-3.44559300
H	5.20633400	2.56761000	-3.53465300
C	-1.70477400	-3.96286800	5.45604600
H	-1.19705400	-4.91425000	5.58716800
C	-1.95115900	-3.13486400	6.58734200
H	-1.65395200	-3.47048500	7.57728400
C	-2.54309000	-1.91241900	6.41863500
H	-2.72161600	-1.25898600	7.26966500
C	-2.08005600	-3.56550300	4.19851100
H	-1.85011800	-4.20006400	3.35188400
N	0.68607500	-2.03233300	1.15861600
S	0.88152500	-3.64569400	1.36326200
C	2.58777700	-3.97606300	0.65041700
O	-0.03385600	-4.44278600	0.54613100
O	1.02998100	-3.92916300	2.79328600
F	2.73548400	-5.29245200	0.49199700
F	2.74246700	-3.36596200	-0.52367100
F	3.53296500	-3.53437900	1.49414700
C	4.72942600	3.16612500	2.04607900
C	4.83062600	4.56523700	1.96235200
C	5.78767000	2.49015300	2.68350500
C	5.93435000	5.25078200	2.47734500
H	4.05041400	5.15720700	1.50024100
C	6.88953900	3.17085100	3.19886900
H	5.77033600	1.41089900	2.77479600
C	6.97226900	4.55998600	3.09663700
H	5.97074800	6.33358900	2.39280600

H	7.68483900	2.60915000	3.68210900
H	7.82955200	5.09333600	3.49814500
C	5.13282800	0.65554300	0.19009000
C	0.52929300	1.68656800	3.10427200
H	0.73217400	2.72886100	2.87488700
H	-0.28874100	1.34120600	2.46232400
H	0.15995100	1.61665300	4.13590900
C	4.88967900	-0.80075500	0.55825700
H	3.82770200	-0.98950300	0.72689500
H	5.19513400	-1.48354000	-0.24266600
H	5.42824700	-1.11340300	1.46343300
C	6.35110600	1.07870800	-0.21277800
C	2.87493100	-1.35556100	3.73228800
H	3.66400700	-1.33240800	2.98154800
H	3.28390900	-0.97161500	4.67599800
H	2.59879900	-2.39975200	3.88143100
C	7.55402900	0.16269200	-0.25950900
H	7.34716600	-0.85570600	0.07325700
H	7.96023300	0.10719900	-1.27981300
H	8.36317500	0.56219400	0.36850800
C	6.68596200	2.48603200	-0.64731300
H	5.81902400	3.13993800	-0.74476200
H	7.37096800	2.95746700	0.07022900
H	7.20943400	2.46967000	-1.61384600
C	0.40981300	-0.94456300	4.20381500
H	0.53150000	-0.55108600	5.22228400
H	-0.53218700	-0.57070300	3.80439900
H	0.33478300	-2.02987700	4.26322700

TS-1-1-7RR-1

1 imaginary frequency

H = -5472.465864

G = -5472.674477

E(M06-2X-DCM) = -5473.444922

C	3.45412100	2.64049700	1.35056200
C	3.11139200	1.69693300	2.58002700
H	3.93047900	0.98644400	2.65572100
H	3.19193000	2.33557000	3.47947400
C	1.82152200	0.98742500	2.89242500
C	2.30587600	3.57276600	0.91113500
H	2.70301600	4.26590600	0.16196900
H	1.96930500	4.19760000	1.74619700
N	1.15087300	2.90368700	0.33789200
C	0.03265100	3.59420200	-0.01148900

N	-0.97690600	2.77153900	-0.46153500
C	-2.27987000	3.07390400	-0.88643100
C	-3.01678300	4.18612600	-0.44688600
C	-2.89268400	2.15812400	-1.75609600
C	-4.32134700	4.37529000	-0.89800100
C	-4.20164100	2.36293900	-2.19050700
H	-2.34381400	1.28355500	-2.09199100
C	-4.92801600	3.47782500	-1.77692200
H	-5.93884800	3.64312000	-2.12902400
C	-4.86220200	1.32178500	-3.04825100
C	-5.13213300	5.52165200	-0.35249400
F	-4.00203700	0.76795100	-3.93442500
F	-5.90354500	1.81432000	-3.74758400
F	-5.34812300	0.29651900	-2.29324200
F	-6.01620100	5.98798500	-1.26209600
F	-4.36439000	6.55471500	0.04091000
F	-5.86066400	5.13652900	0.73008900
S	-0.04393000	5.27684700	0.11064100
C	3.86725600	1.76553600	0.08848900
H	3.51069900	2.31026000	-0.79361600
H	3.27936400	0.84439800	0.11626300
H	-2.56653400	4.89452000	0.23235600
C	1.81167800	-0.36613500	3.30341900
H	-0.73587400	1.77820900	-0.50789900
H	1.17286400	1.90225200	0.15999800
H	1.37997900	-0.95138700	2.21710800
O	-1.68801100	-1.38007700	0.23548700
O	0.26309400	-2.18411000	-1.30018400
P	-0.07559900	-1.28447900	0.00773200
O	0.24106900	0.17222100	-0.12263000
C	-3.61246700	-5.03253500	1.00189300
C	-3.12436800	-4.74309200	-0.26548700
C	-2.60819100	-3.47159800	-0.55973200
C	-2.96716800	-2.79090300	1.75473200
C	-3.58514000	-4.03653000	1.97380700
C	-0.31840300	-1.89300300	-2.54832800
C	-1.60633700	-2.35466200	-2.82229200
C	-2.22186800	-1.98353000	-4.03064200
C	-1.53783000	-1.23836300	-4.98259400
C	-0.21966500	-0.87409200	-4.72885600
C	0.42059200	-1.18209000	-3.51484200
H	-4.03280800	-4.22096900	2.94495600
H	0.34389600	-0.32547600	-5.47715200
C	-2.50830500	-3.32883900	-2.07367900

C	-2.21906000	-4.81199500	-2.47362600
H	-2.45410600	-5.01597100	-3.52287700
H	-1.15430500	-5.01703900	-2.31661100
H	-4.33832300	-1.73985000	-4.46345200
H	-3.71470300	-3.36035600	-4.77571000
C	-2.41211600	-2.56179300	0.47645200
H	-4.03612300	-6.00746100	1.22877900
H	-2.01676300	-0.95372200	-5.91558800
C	-3.06345000	-5.64204500	-1.48140700
H	-4.06530600	-5.85305400	-1.87988100
H	-2.60617000	-6.61076600	-1.25034900
C	-3.63971400	-2.49844000	-4.09804100
C	-3.90879400	-2.89959400	-2.63735400
H	-4.65921300	-3.68764100	-2.52936900
H	-4.26250900	-2.02397100	-2.08313800
C	1.85977400	-0.78735000	-3.39988200
C	2.86893000	-1.77900500	-3.47626600
C	2.20752500	0.58581000	-3.42837300
C	2.58225900	-3.18158800	-3.51142100
C	4.25491100	-1.37832100	-3.57426000
C	3.59265200	0.97031600	-3.57435500
C	3.58283100	-4.11406900	-3.59480300
H	1.54948300	-3.50760800	-3.46966900
C	5.26948800	-2.38412900	-3.65255100
C	4.57689200	-0.01962200	-3.63324300
C	4.94792600	-3.71465400	-3.65793600
H	3.33407100	-5.17161800	-3.61472400
H	6.30647500	-2.06331700	-3.72236000
H	5.61892000	0.27403900	-3.74125400
H	5.72760600	-4.46873900	-3.72223200
C	-3.02446100	-1.77684300	2.85222500
C	-3.69478500	-0.54191900	2.64016500
C	-2.54315200	-2.10724800	4.14751900
C	-4.30576400	-0.18544400	1.39530200
C	-3.82802700	0.39802200	3.73148600
C	-2.73938800	-1.18032900	5.24126800
C	-4.93929900	1.01709500	1.22421100
H	-4.28175000	-0.89054000	0.57371000
C	-4.47266200	1.65516500	3.50344600
C	-3.35441400	0.05066600	4.99948800
C	-5.00685300	1.96641700	2.28276700
H	-5.39603000	1.24503500	0.26687200
H	-4.53671000	2.35619900	4.33249400
H	-3.48430200	0.74981800	5.82349800

H	-5.48216500	2.92762900	2.11148100
C	1.59575000	2.95546700	-3.41102400
H	0.83886800	3.72970100	-3.32404900
C	1.23603600	1.63476600	-3.33275000
H	0.19493100	1.36887400	-3.19253900
C	2.95856500	3.32587400	-3.59730200
H	3.22384700	4.37671600	-3.67353400
C	3.92493500	2.35852300	-3.67138700
H	4.96953500	2.62802700	-3.80602600
C	-1.42495100	-3.62642100	5.70724600
H	-0.89041000	-4.55466800	5.88830400
C	-1.66089700	-2.72824800	6.78619900
H	-1.32801800	-2.98778700	7.78760200
C	-2.28915300	-1.53509800	6.55214000
H	-2.46182800	-0.82949600	7.36171500
C	-1.84380600	-3.32525100	4.43695600
H	-1.62122800	-4.01121600	3.62934700
N	0.80215800	-1.95958000	1.23574100
S	1.02892900	-3.55894100	1.51170600
C	2.70975100	-3.91427100	0.75110200
O	0.09373700	-4.40701500	0.77214200
O	1.23786000	-3.76858000	2.94687600
F	2.84867200	-5.23528200	0.62644600
F	2.82783500	-3.34007700	-0.44558700
F	3.68198700	-3.45203400	1.55093900
C	4.61335000	3.53296200	1.88353600
C	4.57942800	4.93675700	1.84373500
C	5.73782800	2.93978900	2.48924200
C	5.61943500	5.70696600	2.37229500
H	3.74309200	5.46530900	1.40291100
C	6.77573200	3.70528600	3.01728400
H	5.82716700	1.86032800	2.52796900
C	6.72363500	5.09862600	2.96249800
H	5.55381500	6.79046000	2.32035500
H	7.62796900	3.20679100	3.47196800
H	7.53070700	5.69817400	3.37445000
C	5.33670700	1.46748900	-0.16660000
C	0.56453600	1.79262000	3.04340300
H	0.68569100	2.83476200	2.76173600
H	-0.25174100	1.36391800	2.45147500
H	0.24122700	1.74572300	4.09173600
C	6.14163400	2.65060600	-0.69629500
H	5.52980000	3.55419400	-0.74744700
H	7.00749200	2.89074200	-0.07077300

H	6.51229300	2.45386500	-1.71003400
C	5.89203100	0.24002400	-0.07493900
C	3.13261500	-1.08616500	3.61101700
H	3.86033500	-1.03333600	2.80092600
H	3.59020700	-0.66281200	4.51473200
H	2.92881600	-2.14095000	3.79828600
C	7.34274900	-0.01906200	-0.42047100
H	7.91748900	0.88687400	-0.61910600
H	7.84207300	-0.56085600	0.39486000
H	7.41706800	-0.66690200	-1.30617700
C	5.16904900	-1.02357200	0.31771900
H	4.10497200	-0.88879700	0.51181600
H	5.25306100	-1.77345800	-0.47998900
H	5.62278400	-1.47659100	1.21030600
C	0.68755800	-0.79477100	4.25902400
H	0.85815000	-0.35650600	5.25182000
H	-0.30053000	-0.49058500	3.91687800
H	0.68133300	-1.87936900	4.35737600

TS-1-2-7SS

l imaginary frequency

H = -5472.463010

G = -5472.675620

E(M06-2X-DCM) = -5473.449034

O	-1.32731200	-1.42253400	-1.63045400
O	-3.10046500	-0.62713600	0.11680100
P	-1.50859900	-0.81655800	-0.13598400
O	-0.95156500	0.61931300	-0.00799100
N	-0.97121800	-1.93281300	0.87232800
S	0.59645200	-2.23185000	1.00886200
C	0.74040200	-3.99695700	0.41255400
F	0.22747600	-4.11195600	-0.81251800
F	0.08543500	-4.82269000	1.23790600
F	2.03106100	-4.33776900	0.38815000
C	-0.11697900	4.48434300	0.51474000
C	-0.15882000	4.01099900	2.02224100
H	-1.07259900	4.43148700	2.45418100
H	0.68521700	4.50077100	2.51665800
C	-0.11256400	2.55661600	2.44774300
C	1.12712200	3.88290000	-0.22276400
H	0.95965200	3.92143500	-1.30229100
H	1.99334300	4.50793300	-0.00696700
N	1.53345200	2.52808500	0.13435700
C	2.84407200	2.22018800	0.44222500

N	3.07025900	0.87526000	0.53541500
C	4.27820000	0.19209800	0.82313700
C	5.20216600	0.61644100	1.78710500
C	4.50551800	-1.00900000	0.14144900
C	6.34806900	-0.14205700	2.02642900
C	5.65570000	-1.75523500	0.39399500
H	3.77708300	-1.36336400	-0.57646600
C	6.59320300	-1.32683700	1.33095500
H	7.49110800	-1.90244400	1.51967400
C	5.90319000	-2.99207800	-0.42501900
C	7.30264600	0.28491600	3.11051400
F	6.37379600	-2.67858700	-1.66589900
F	6.81591000	-3.80899500	0.13931800
F	4.77432700	-3.70859200	-0.61865600
F	8.57431600	-0.08134000	2.82976800
F	7.29595900	1.62094000	3.29792000
F	6.98877600	-0.28106500	4.30080200
S	4.01980300	3.39834900	0.72800900
H	5.03588500	1.53246700	2.33425700
C	-1.21522200	1.69213900	2.45119400
H	2.32199800	0.23677500	0.25407400
O	1.41724700	-1.46205400	0.03793800
H	0.95248700	1.76963400	-0.21770300
O	1.03080300	-2.24864900	2.40779400
H	-0.96628400	1.20545800	1.19585300
C	-5.76944000	-3.81223400	-0.45639700
C	-5.31121900	-3.06882600	-1.53710100
C	-4.46478400	-1.96218400	-1.34956100
C	-4.52007400	-2.35964500	1.06260100
C	-5.39503500	-3.43324900	0.83060000
C	-1.65140000	-0.73227000	-2.80329500
C	-2.98960100	-0.50863100	-3.11256900
C	-3.30763000	0.38042000	-4.15056800
C	-2.30600700	0.87843700	-4.97889100
C	-0.98887900	0.45722300	-4.77963400
C	-0.62092000	-0.34848300	-3.68730100
H	-5.77850700	-3.97551200	1.68971100
H	-0.21542300	0.75841300	-5.47965700
C	-4.25926200	-1.23718800	-2.67894200
C	-4.50863600	-2.42691100	-3.67560900
H	-3.58348200	-3.00814700	-3.76260000
H	-4.77906000	-2.08108500	-4.67722200
H	-5.24140400	0.17741800	-5.12106300
H	-5.06264000	1.67262600	-4.21353900

C	-4.02222500	-1.66951000	-0.05986300
H	-6.42175600	-4.66834700	-0.60781700
H	-2.54502200	1.54552500	-5.80346100
C	-5.59408400	-3.28723000	-3.00469200
H	-5.53788700	-4.34304400	-3.29241700
H	-6.60289000	-2.94052200	-3.26991000
C	-4.80554900	0.60700300	-4.20904500
C	-5.31776700	-0.11715100	-2.93880600
H	-5.32156600	0.57318600	-2.08750800
H	-6.33064900	-0.51643800	-3.05025500
C	0.77321000	-0.87898400	-3.56057100
C	1.88201900	-0.00746500	-3.42314200
C	0.98254500	-2.28114100	-3.65819000
C	1.75752600	1.41839000	-3.37050400
C	3.21659000	-0.55701500	-3.32970700
C	2.31770100	-2.81440000	-3.51822700
C	2.85661600	2.23117300	-3.25715700
H	0.77032300	1.85798700	-3.43224100
C	4.33498300	0.32501600	-3.19612900
C	3.39585400	-1.94195300	-3.35382700
C	4.16677500	1.68245800	-3.16419800
H	2.73043600	3.31016700	-3.22693100
H	5.32451500	-0.11622100	-3.10756500
H	4.39720000	-2.34977300	-3.24462900
H	5.02079400	2.34336600	-3.05242100
C	-4.26225700	-1.96497900	2.48486600
C	-3.48080300	-2.78961300	3.32854200
C	-4.93847900	-0.83692800	3.01371800
C	-2.77626100	-3.94075300	2.85076600
C	-3.37300300	-2.47119600	4.73527600
C	-4.80356100	-0.51872200	4.41756300
C	-2.04230000	-4.72651400	3.69947000
H	-2.80736300	-4.17125100	1.79291600
C	-2.59795400	-3.31989200	5.58624000
C	-4.02976200	-1.34485700	5.23778000
C	-1.95517600	-4.41938200	5.08714100
H	-1.50278500	-5.58335100	3.30775900
H	-2.53034000	-3.06715900	6.64172400
H	-3.94367500	-1.10972400	6.29690300
H	-1.36563900	-5.05508300	5.74187800
C	0.17458500	-4.56354800	-4.01182400
H	-0.64375800	-5.24476300	-4.23008400
C	-0.06640800	-3.21671700	-3.93272200
H	-1.07086300	-2.84689200	-4.10236900

C	1. 48303200	-5. 08454700	-3. 80887900
H	1. 65073800	-6. 15707500	-3. 85392400
C	2. 52326100	-4. 22844200	-3. 57170400
H	3. 53255400	-4. 60361600	-3. 42286900
C	-6. 43063400	1. 08625000	2. 76810800
H	-7. 07237000	1. 70304700	2. 14451000
C	-6. 27206600	1. 41006300	4. 14575100
H	-6. 78769300	2. 27226600	4. 55986300
C	-5. 48340300	0. 62477500	4. 94341900
H	-5. 36592300	0. 85024500	6. 00095200
C	-5. 78971800	0. 00309400	2. 22424700
H	-5. 93282800	-0. 23328800	1. 17566400
C	1. 16203200	2. 11134800	3. 10669800
H	1. 43235700	1. 08063400	2. 86501200
H	2. 00344000	2. 76556600	2. 87836300
H	0. 99238100	2. 13258400	4. 19523500
C	-1. 15357900	0. 42258000	3. 30940100
H	-0. 24651600	-0. 16953300	3. 18439100
H	-1. 23892600	0. 69533700	4. 37003300
H	-1. 99465100	-0. 22927400	3. 07041000
C	0. 04435100	6. 02566700	0. 50497700
C	-0. 33265200	6. 84197100	1. 58326000
C	0. 55498300	6. 67308300	-0. 63488300
C	-0. 20099500	8. 23162500	1. 53228300
H	-0. 73424200	6. 41006200	2. 49298100
C	0. 68906500	8. 05974000	-0. 69094200
H	0. 85710000	6. 09465400	-1. 50000500
C	0. 31096600	8. 85062700	0. 39441600
H	-0. 49838800	8. 82623200	2. 39212800
H	1. 09516600	8. 52005000	-1. 58786300
H	0. 41878800	9. 93105900	0. 35448200
C	-1. 48753400	4. 12541800	-0. 17814300
H	-1. 59880000	3. 03592100	-0. 16469600
H	-2. 26778700	4. 52596100	0. 47290800
C	-1. 74349300	4. 59980300	-1. 60096100
C	-2. 44571400	5. 71574300	-1. 89631700
C	-1. 23323600	3. 67802700	-2. 69805200
H	-0. 34973200	4. 07709100	-3. 21696900
H	-0. 95887000	2. 70270400	-2. 28760800
H	-1. 98961800	3. 48890600	-3. 46591200
C	-2. 70532100	6. 16347900	-3. 31859600
H	-2. 37599500	7. 20318300	-3. 45280600
H	-2. 19918100	5. 55892700	-4. 07284200
H	-3. 78228500	6. 15279200	-3. 54127800

C	-3.04864700	6.66627600	-0.88813100
H	-3.02991500	6.30256900	0.13996500
H	-2.51644000	7.62690600	-0.89956300
H	-4.09365100	6.88148400	-1.15141700
C	-2.65363300	2.20263500	2.32832400
H	-2.73639600	3.20351300	1.91165500
H	-3.25443100	1.52938700	1.71200900
H	-3.10821800	2.20841100	3.32682900

TS-1-2-7SS-1

l imaginary frequency

H = -5472.458992

G = -5472.670617

E(M06-2X-DCM) = -5473.443575

O	1.64287300	-1.13714700	1.63077000
O	3.38959600	0.04365100	0.08472300
P	1.84263600	-0.43021400	0.18523700
O	1.04354600	0.88383800	0.05372000
N	1.59652700	-1.57382300	-0.90535600
S	0.14002400	-2.15942700	-1.19554200
C	0.33178100	-3.96972700	-0.77517100
F	0.80841100	-4.10888500	0.46119100
F	1.17320100	-4.55561100	-1.63537200
F	-0.86297200	-4.55909000	-0.86213400
C	-1.00032700	4.31065800	-0.59999200
C	-0.81508200	3.76685400	-2.07519900
H	-0.18945000	4.49981500	-2.59956900
H	-1.80832700	3.81042100	-2.52578300
C	-0.25768400	2.40400900	-2.44712500
C	-1.56840800	3.20110700	0.36745700
H	-0.85191200	3.04302900	1.17337100
H	-2.49654900	3.54735400	0.81387800
N	-1.84475100	1.87661300	-0.18468100
C	-3.11491100	1.45980600	-0.51555800
N	-3.20083600	0.09786900	-0.63984500
C	-4.29667000	-0.75661600	-0.87532100
C	-5.51895700	-0.37524400	-1.44719800
C	-4.10683900	-2.10240200	-0.51403500
C	-6.52565800	-1.32735800	-1.62232400
C	-5.12816800	-3.03098600	-0.68697900
H	-3.15693000	-2.41698700	-0.09720400
C	-6.35263500	-2.65614300	-1.24051600
H	-7.14776400	-3.37953400	-1.37155600
C	-4.92340300	-4.43367000	-0.18360400

C	-7.80543000	-0.91405600	-2.30258200
F	-5.19536800	-4.52437600	1.15148100
F	-5.73051400	-5.32184400	-0.79936500
F	-3.65155600	-4.85403700	-0.34114900
F	-8.84595700	-1.69514800	-1.93159200
F	-8.13826900	0.36350500	-2.02477000
F	-7.70498100	-1.01066600	-3.64961300
S	-4.35895400	2.56341600	-0.77887800
H	-5.68514000	0.65283800	-1.73255600
C	1.08919100	2.02871500	-2.39179800
H	-2.35029400	-0.42719300	-0.42613700
O	-0.88946500	-1.66610100	-0.24055800
H	-1.17713000	1.16144400	0.09404200
O	-0.20110400	-2.12604800	-2.62187300
H	0.93721300	1.46178900	-1.14206400
C	6.47314800	-2.75955800	0.57283900
C	5.82920700	-2.21660400	1.67780200
C	4.84424200	-1.22499400	1.52711800
C	5.13222400	-1.33794500	-0.89778200
C	6.14318900	-2.29238600	-0.69702900
C	1.79773300	-0.50210400	2.86868300
C	3.07591300	-0.15345100	3.29735000
C	3.21411200	0.66647800	4.42819700
C	2.10818700	0.96877600	5.21650800
C	0.86722700	0.42688000	4.87779900
C	0.67005100	-0.30824000	3.69445000
H	6.66766300	-2.67276900	-1.56833700
H	0.01723000	0.57631600	5.53637800
C	4.45318400	-0.67740300	2.89811700
C	4.79222400	-1.92301500	3.79337600
H	3.95162700	-2.62493000	3.74693700
H	4.94206300	-1.65343600	4.84258500
H	5.08841900	0.58992000	5.52385200
H	4.78839800	2.13984500	4.75014700
C	4.45441900	-0.85830100	0.23973300
H	7.23422700	-3.52598400	0.69417000
H	2.21086800	1.57876600	6.11050700
C	6.03110900	-2.55766100	3.13568000
H	6.09836800	-3.63744700	3.30966200
H	6.96125500	-2.11711400	3.52144700
C	4.66479200	1.05780700	4.62495700
C	5.34284500	0.53079200	3.33737800
H	5.31105600	1.29744700	2.55458900
H	6.38945900	0.24773100	3.48556200

C	-0.65591100	-0.94148200	3.41223300
C	-1.83085300	-0.15372500	3.30931600
C	-0.74581300	-2.35786900	3.34519900
C	-1.83380700	1.27382300	3.43145700
C	-3.10617300	-0.79808400	3.08250800
C	-2.01875800	-2.98005900	3.06158800
C	-2.99849600	1.99628700	3.38214100
H	-0.89113400	1.78872600	3.57179200
C	-4.29415900	-0.00488700	3.01502700
C	-3.16099300	-2.18583300	2.93300100
C	-4.25051000	1.35360000	3.17103200
H	-2.96611700	3.07679500	3.49487400
H	-5.23898100	-0.51212600	2.83736200
H	-4.11516800	-2.66183400	2.72148800
H	-5.15925300	1.94509700	3.11658100
C	4.91639100	-0.83718200	-2.29236700
C	4.39523300	-1.70088700	-3.28580700
C	5.38067900	0.45639500	-2.64126200
C	3.88187800	-3.00404300	-2.98799300
C	4.35791700	-1.26303300	-4.66347000
C	5.31467600	0.88878600	-4.01954600
C	3.39547200	-3.81875900	-3.97619500
H	3.85116400	-3.33117500	-1.95600100
C	3.85041300	-2.14907500	-5.66483100
C	4.81604300	0.01587400	-4.99080800
C	3.38746700	-3.39347300	-5.33506100
H	2.99235000	-4.79371900	-3.71929500
H	3.83674300	-1.80578300	-6.69658500
H	4.78556200	0.34016100	-6.02925300
H	2.99866900	-4.05615700	-6.10323800
C	0.23783100	-4.59089600	3.51585700
H	1.09847600	-5.22288400	3.71891400
C	0.36360400	-3.22847500	3.59272900
H	1.31949500	-2.79845500	3.86838900
C	-1.00366000	-5.19127800	3.16550700
H	-1.07693400	-6.27217500	3.08356700
C	-2.10093900	-4.40386300	2.94756800
H	-3.05940500	-4.84139000	2.68314600
C	6.38247800	2.61181100	-2.06222600
H	6.80784900	3.27945900	-1.31765900
C	6.29268000	3.04051400	-3.41715500
H	6.64365500	4.03094600	-3.69375800
C	5.77772700	2.19750400	-4.36499900
H	5.71690200	2.50500100	-5.40649200

C	5.94688500	1.36625900	-1.69020600
H	6.03699400	1.05490200	-0.65563800
C	-1.23375100	1.48513900	-3.13378700
H	-1.10368400	0.43251500	-2.87045900
H	-2.26925500	1.77577100	-2.96060400
H	-1.03743300	1.54735000	-4.21599400
C	1.55963200	0.83564300	-3.23079600
H	0.90650900	-0.03475600	-3.20161400
H	1.65819500	1.15447500	-4.27735700
H	2.54591500	0.51362700	-2.89550100
C	-1.96051500	5.52746400	-0.67369800
C	-2.07789500	6.31964500	-1.82783900
C	-2.69841400	5.93631700	0.45044900
C	-2.90442100	7.44484000	-1.86662700
H	-1.52751000	6.07132600	-2.72841000
C	-3.52763300	7.05633600	0.41703300
H	-2.61862100	5.39185300	1.38469800
C	-3.64057500	7.81861300	-0.74498700
H	-2.97154200	8.02426900	-2.78382900
H	-4.08782600	7.33049400	1.30722300
H	-4.29012100	8.68906100	-0.77462400
C	0.40041800	4.80430800	-0.05740700
H	1.03819600	3.92304900	0.02499800
H	0.83353300	5.43351300	-0.84650500
C	0.47803900	5.61701600	1.22808600
C	0.92869100	5.11748100	2.40014700
C	0.19878700	7.11039600	1.07946300
H	1.09437000	7.70013600	1.31502300
H	-0.09770900	7.36018800	0.05913600
H	-0.60524200	7.46389300	1.73310100
C	1.08416400	5.97834900	3.63612500
H	2.14656700	6.08765000	3.90040500
H	0.66354200	6.97937600	3.53114200
H	0.60198500	5.50132500	4.50049400
C	1.40035100	3.70231800	2.63896100
H	1.32072200	3.03326400	1.78124600
H	2.45492600	3.71031500	2.95182000
H	0.85200900	3.24192100	3.47091800
C	2.22927500	3.03201700	-2.19993900
H	1.89932700	4.03615900	-1.94579700
H	2.92974700	2.69398700	-1.42950000
H	2.79908500	3.09001500	-3.13506000

l imaginary frequency

H = -5472.463334

G = -5472.675289

E(M06-2X-DCM) = -5473.447255

O	1.31809000	-1.28161000	1.79101200
O	3.10074500	-0.79266900	-0.05275600
P	1.49905100	-0.84379000	0.23520500
O	1.01420100	0.59103900	-0.01804900
N	0.89529400	-2.03275500	-0.64700700
S	-0.68235200	-2.25664200	-0.77409500
C	-0.90713600	-3.96374900	-0.04988900
F	-0.45772500	-3.99407200	1.20534100
F	-0.23546500	-4.87011400	-0.77295000
F	-2.20554400	-4.27329300	-0.06418300
C	0.07429700	4.43265100	-0.90326500
C	0.40373800	3.85414100	-2.33605500
H	1.41962700	4.16268200	-2.59345600
H	-0.27500600	4.36193800	-3.02831800
C	0.25576800	2.38520600	-2.66489600
C	-1.38334600	4.04379700	-0.50950100
H	-1.60275500	4.46182600	0.47891600
H	-2.07720500	4.52129800	-1.20192600
N	-1.71286600	2.62072600	-0.52183400
C	-2.99924700	2.19530300	-0.79595700
N	-3.17036500	0.84714500	-0.64289800
C	-4.35124700	0.07754700	-0.80157400
C	-5.28711300	0.29436100	-1.82251200
C	-4.53751600	-0.99558500	0.07742900
C	-6.40515800	-0.53256500	-1.92262300
C	-5.65713300	-1.81947200	-0.04370800
H	-3.79821500	-1.19500200	0.84298800
C	-6.60755100	-1.59053000	-1.03508700
H	-7.48200100	-2.22352000	-1.12072200
C	-5.83456600	-2.93726100	0.94734900
C	-7.37350000	-0.33194000	-3.05881400
F	-6.13888100	-2.46389500	2.19013800
F	-6.82842200	-3.78038000	0.60104700
F	-4.70817300	-3.66829800	1.08960900
F	-8.63247000	-0.68410100	-2.70995600
F	-7.41069000	0.95023600	-3.47633600
F	-7.04264600	-1.08692900	-4.13390400
S	-4.20884200	3.25205600	-1.31470600
H	-5.14910400	1.10491600	-2.52224400
C	1.29621100	1.44833800	-2.55024400

H	-2.38831600	0.29037200	-0.28878800
O	-1.46940700	-1.37619300	0.12787400
H	-1.14353500	2.01283500	0.06304100
O	-1.11520400	-2.36001700	-2.17059400
H	1.01046700	1.08960000	-1.30992300
C	5.42581500	-4.20744700	0.68042300
C	5.06844700	-3.35656500	1.71934100
C	4.35111900	-2.17437400	1.47018800
C	4.33029000	-2.70918300	-0.91346600
C	5.08414900	-3.85870000	-0.62437900
C	1.75339900	-0.49403100	2.86101400
C	3.11667000	-0.42017700	3.13469000
C	3.57647100	0.52519000	4.06351900
C	2.67232800	1.25613000	4.82833800
C	1.30565100	1.01675100	4.67334700
C	0.80643000	0.15112900	3.68288100
H	5.39771300	-4.48636700	-1.45317200
H	0.59550500	1.51326300	5.32751300
C	4.26859900	-1.34236100	2.74749800
C	4.39382100	-2.47967000	3.82283000
H	3.40604500	-2.93168300	3.96916500
H	4.73290500	-2.10122800	4.79151800
H	5.47630200	0.13576600	5.03971500
H	5.49630600	1.55788600	4.00528400
C	3.92109800	-1.90804100	0.17081800
H	5.97904800	-5.12240100	0.87593200
H	3.01963000	1.96951300	5.57170700
C	5.34707500	-3.51470400	3.19624700
H	5.16061900	-4.53385500	3.55317800
H	6.39693700	-3.28631200	3.42820500
C	5.09103000	0.54331800	4.09513500
C	5.47175500	-0.35411100	2.89330100
H	5.54468600	0.25087000	1.98216500
H	6.42569300	-0.87357200	3.02706100
C	-0.65942700	-0.13571700	3.59944500
C	-1.59096900	0.91040200	3.37956300
C	-1.12338700	-1.45742400	3.83493200
C	-1.20484600	2.27733500	3.19200400
C	-3.00660800	0.61602900	3.35428700
C	-2.53813500	-1.74212700	3.75876900
C	-2.13877600	3.27139800	3.04137400
H	-0.15029500	2.52491200	3.18910500
C	-3.94474400	1.67809100	3.16172700
C	-3.43946300	-0.70164500	3.51979800

C	-3.53047200	2.97429800	3.01978500
H	-1.81615300	4.30434900	2.93673000
H	-5.00248300	1.42900100	3.13498200
H	-4.50209600	-0.92338600	3.46443100
H	-4.25249300	3.77265000	2.87799300
C	4.10795500	-2.36487700	-2.35435800
C	3.26483900	-3.16506300	-3.16226700
C	4.87122900	-1.31984900	-2.93427200
C	2.46139000	-4.22439800	-2.63130500
C	3.18964100	-2.91225800	-4.58442700
C	4.76527800	-1.06215800	-4.35311600
C	1.66599600	-4.98782700	-3.44436000
H	2.46263500	-4.39639200	-1.56229300
C	2.35178900	-3.73809400	-5.39753700
C	3.93486800	-1.86768600	-5.13759600
C	1.61494200	-4.75089700	-4.84742400
H	1.04917200	-5.76971900	-3.01208500
H	2.31195900	-3.53741400	-6.46558700
H	3.87226400	-1.68072500	-6.20795200
H	0.97718900	-5.36861800	-5.47361900
C	-0.74396200	-3.80497500	4.40558900
H	-0.06070500	-4.60408000	4.68094000
C	-0.25881600	-2.54143600	4.19197300
H	0.80129800	-2.35217500	4.31294900
C	-2.13150500	-4.08832000	4.26661000
H	-2.49339400	-5.10154000	4.41747500
C	-3.00262900	-3.08073800	3.95557400
H	-4.06573300	-3.27416400	3.84662100
C	6.50304500	0.49649400	-2.77424800
H	7.18831600	1.09284100	-2.17760200
C	6.37192300	0.76396200	-4.16673300
H	6.95097700	1.56446900	-4.61915800
C	5.52967900	0.00054600	-4.92984500
H	5.43198300	0.18165200	-5.99788900
C	5.78235800	-0.50852200	-2.18226000
H	5.90661000	-0.70415100	-1.12306400
C	-1.02177100	1.97850600	-3.33779900
H	-1.37727600	0.99669000	-3.01540400
H	-1.82256500	2.70712200	-3.21165100
H	-0.80399700	1.88314500	-4.41431200
C	1.18320000	0.12931200	-3.32403800
H	0.23637900	-0.39459400	-3.18514900
H	1.31722100	0.31868600	-4.39739900
H	1.97242100	-0.55364400	-3.00936200

C	0.04840300	5.98088400	-0.97476900
C	0.27863100	6.71971800	-2.14462400
C	-0.25012500	6.70838600	0.19174100
C	0.20587700	8.11574500	-2.15328200
H	0.52786300	6.22520600	-3.07652500
C	-0.33180900	8.09889100	0.18691100
H	-0.41991800	6.18493500	1.12627000
C	-0.10446200	8.81387600	-0.98969700
H	0.39132900	8.65159400	-3.08041100
H	-0.57166500	8.62329700	1.10809300
H	-0.16674200	9.89852100	-0.99691900
C	1.09493100	3.94611800	0.20757700
H	0.51272600	3.73179800	1.10449100
H	1.49354700	2.96977500	-0.08608900
C	2.27281700	4.84355400	0.58243100
C	2.49637600	5.26361300	1.84708600
C	3.24710000	5.15531100	-0.53755000
H	3.92281600	4.31101500	-0.73391800
H	2.72229600	5.37533600	-1.47147600
H	3.86802100	6.02754300	-0.32777200
C	3.72935700	6.03608700	2.27258000
H	4.12738900	5.61747800	3.20681500
H	4.54067300	6.02740600	1.54369600
H	3.47923200	7.08517800	2.48800500
C	1.57716200	5.02259300	3.02533300
H	0.56091400	4.73475000	2.75277700
H	1.97690500	4.23730200	3.68282500
H	1.50496200	5.93265100	3.63576400
C	2.75234600	1.89726400	-2.39718300
H	2.86668100	2.82524800	-1.84171400
H	3.33185800	1.12660200	-1.88556800
H	3.19693400	2.03144200	-3.39175700

TS-1-2-7SS-3

l imaginary frequency

H = -5472.463129

G = -5472.675286

E(M06-2X-DCM) = -5473.446891

O	-1.40859000	-1.38091300	-1.69863100
O	-3.17517200	-0.62445700	0.06496100
P	-1.57620700	-0.72919700	-0.21948100
O	-1.06910200	0.72089800	-0.16860500
N	-0.96984200	-1.79057200	0.81151600
S	0.60494400	-2.03055500	0.92649000

C	0.76483300	-3.84873000	0.52793600
F	0.25374700	-4.10297400	-0.67749600
F	0.11514700	-4.58517200	1.43924700
F	2.05747700	-4.18145600	0.54099300
C	0.36383100	4.59726300	0.30881100
C	0.01486500	4.17876400	1.78743100
H	-0.93983400	4.64827500	2.04162700
H	0.78128200	4.62982100	2.42363200
C	-0.03763000	2.73238700	2.23645200
C	1.73403700	3.98074300	-0.13559800
H	1.88626500	4.21596500	-1.19455200
H	2.53124300	4.48471300	0.41062000
N	1.95506700	2.55516400	0.07883400
C	3.19912600	2.07875000	0.45123600
N	3.27840400	0.71581800	0.44038100
C	4.39514800	-0.11105200	0.71823200
C	5.29878200	0.12819700	1.76317600
C	4.54621400	-1.25877000	-0.06634400
C	6.35413800	-0.75603100	1.97886900
C	5.60573600	-2.13653100	0.16739100
H	3.82993200	-1.46723900	-0.85224400
C	6.52549400	-1.89005300	1.18215600
H	7.35530100	-2.56467500	1.35268300
C	5.74836600	-3.33196400	-0.73288300
C	7.28810100	-0.52970700	3.13879500
F	6.01990800	-2.95654600	-2.01566300
F	6.74367300	-4.15581900	-0.34808600
F	4.61201500	-4.06065100	-0.78578100
F	8.54474200	-0.94337200	2.85437400
F	7.35779400	0.76995300	3.49233800
F	6.89276500	-1.21733200	4.23693800
S	4.46683500	3.09326600	0.91418700
H	5.18401500	0.99915800	2.39087900
C	-1.19660400	1.94283600	2.21701700
H	2.46757000	0.17852600	0.12081700
O	1.37912200	-1.35701900	-0.14952100
H	1.36140900	1.91556600	-0.44338200
O	1.09211000	-1.88129300	2.30197300
H	-0.98056000	1.37797400	1.02084200
C	-5.45021400	-4.15209000	-0.00764400
C	-5.10807300	-3.50623600	-1.18920500
C	-4.41673700	-2.28267800	-1.17028900
C	-4.38165800	-2.36085400	1.27107200
C	-5.11698500	-3.55617200	1.20631800

C	-1.88371800	-0.79688900	-2.87588100
C	-3.24921200	-0.82907700	-3.14565900
C	-3.74873000	-0.08857700	-4.22840800
C	-2.87845900	0.53327300	-5.11807100
C	-1.50294100	0.39056000	-4.93011800
C	-0.96782100	-0.26310700	-3.80573900
H	-5.41868200	-4.02170800	2.13970800
H	-0.81435200	0.79715300	-5.66453900
C	-4.36311800	-1.70534900	-2.58276900
C	-4.44999900	-3.02846700	-3.42248700
H	-3.44903800	-3.47132500	-3.48094800
H	-4.79576400	-2.85111100	-4.44499700
H	-5.62974200	-0.73339800	-5.09969500
H	-5.71010400	0.85643100	-4.35213100
C	-3.98794200	-1.77025100	0.05400700
H	-5.98459500	-5.09841800	-0.02530700
H	-3.25729800	1.08834300	-5.97260500
C	-5.37690400	-3.95086500	-2.60843900
H	-5.16032700	-5.01382400	-2.76344300
H	-6.43162400	-3.80115000	-2.87901600
C	-5.26249700	-0.13914800	-4.25191800
C	-5.60497000	-0.80872900	-2.90024800
H	-5.70055700	-0.04647100	-2.11821400
H	-6.53799100	-1.37996900	-2.92450700
C	0.50849000	-0.46961700	-3.68754100
C	1.39393700	0.63638300	-3.64401400
C	1.02561200	-1.79158500	-3.71816700
C	0.94875900	1.99870300	-3.67616600
C	2.82144700	0.40739700	-3.58309700
C	2.45158800	-2.00368300	-3.62126900
C	1.83962300	3.04216800	-3.69943300
H	-0.11534500	2.20221400	-3.70646200
C	3.71297900	1.52569400	-3.57184500
C	3.30880400	-0.90197900	-3.54939700
C	3.24308400	2.80913000	-3.64232100
H	1.47026200	4.06286900	-3.76334100
H	4.78076000	1.33013500	-3.51545800
H	4.38115700	-1.07039400	-3.47877900
H	3.93230300	3.64841700	-3.64463200
C	-4.15731000	-1.75795400	2.62332600
C	-3.32500700	-2.40941100	3.56563200
C	-4.90746400	-0.61550800	3.00195300
C	-2.52092800	-3.54651300	3.23309800
C	-3.25749200	-1.91230000	4.92201400

C	-4.80933400	-0.11496200	4.35501600
C	-1.73316200	-4.15828300	4.17225900
H	-2.51273900	-3.90049500	2.20992600
C	-2.43073700	-2.58798500	5.87349000
C	-3.99724400	-0.78125800	5.27720100
C	-1.69331900	-3.68274300	5.51375700
H	-1.11420700	-5.00322400	3.88604400
H	-2.39841800	-2.20507600	6.89082700
H	-3.94190100	-0.41103600	6.29917000
H	-1.06326000	-4.18420900	6.24316000
C	0.73699300	-4.21241900	-3.90880000
H	0.08406900	-5.07109700	-4.04111000
C	0.20248000	-2.95109600	-3.88512600
H	-0.86604800	-2.82509100	-4.01287100
C	2.13741000	-4.41452600	-3.76128300
H	2.54097800	-5.42315200	-3.76479500
C	2.96955900	-3.33726000	-3.62692800
H	4.04079800	-3.47268400	-3.51712400
C	-6.50282400	1.17238200	2.50748900
H	-7.16965000	1.66810300	1.80693700
C	-6.38128100	1.67562200	3.83390400
H	-6.94904300	2.55277900	4.13211500
C	-5.56101400	1.04315000	4.72880000
H	-5.46937400	1.40652700	5.74984700
C	-5.79599700	0.06729500	2.10880900
H	-5.91413000	-0.30776500	1.09848800
C	1.18095700	2.21818500	2.94722300
H	1.40395700	1.17421000	2.71153400
H	2.06802900	2.82413300	2.76306100
H	0.96245000	2.24279800	4.02735700
C	-1.25571100	0.72102100	3.14179200
H	-0.38007800	0.07299600	3.08990700
H	-1.37560100	1.05413200	4.18141500
H	-2.12274700	0.11017000	2.89211100
C	0.65365800	6.12229500	0.24035600
C	0.74782600	6.95735700	1.36333600
C	0.90705700	6.70879800	-1.01314200
C	1.06888100	8.31154400	1.24207000
H	0.55383100	6.57572000	2.35913900
C	1.23298400	8.05814700	-1.13943800
H	0.84367100	6.10961400	-1.91588400
C	1.31499600	8.87157300	-0.00905000
H	1.12511400	8.92602900	2.13668600
H	1.42199400	8.47207500	-2.12643500

H	1.56713300	9.92406400	-0.10321000
C	-0.75314000	4.18239600	-0.70244500
H	-0.33536600	4.35574200	-1.70316800
H	-0.85441600	3.09668000	-0.63203400
C	-2.16225600	4.81368700	-0.66802700
C	-3.18062400	4.19446400	-1.30957900
C	-2.34861400	6.16587500	-0.01071100
H	-1.95851500	6.19728600	1.01122400
H	-1.81802500	6.95245300	-0.55927800
H	-3.39766100	6.45795600	0.03886400
C	-4.60286700	4.71214400	-1.38727400
H	-5.30750400	3.88777800	-1.21343300
H	-4.84401600	5.50180600	-0.67461100
H	-4.82195800	5.09692000	-2.39400800
C	-3.04001200	2.89435200	-2.06908600
H	-2.01424900	2.55946500	-2.21532900
H	-3.57424000	2.08403000	-1.55441800
H	-3.50168600	2.98975500	-3.06103600
C	-2.57716200	2.56573500	1.99660100
H	-2.58531500	3.37566900	1.26858300
H	-3.27726200	1.80230200	1.64852300
H	-2.96189500	2.94392900	2.95327200

TS-1-2-7SR

l imaginary frequency

H = -5472.467566

G = -5472.678698

E(M06-2X-DCM) = -5473.451811

O	-1.71283300	-1.28057700	-1.54551300
O	-3.28544600	0.11983800	0.00606500
P	-1.75842700	-0.41050600	-0.17194700
O	-0.90313900	0.86373500	-0.27540000
N	-1.47108700	-1.43632000	1.02046800
S	-0.00762000	-2.02595100	1.27319400
C	-0.28470800	-3.86709900	1.12057600
F	-0.82334000	-4.15755800	-0.06435800
F	-1.10803800	-4.29662900	2.08697300
F	0.88848300	-4.49246200	1.24011700
C	0.95768700	4.50671400	-0.39093900
C	0.67954200	4.37461500	1.15740800
H	-0.14031900	5.06146900	1.39413600
H	1.57370300	4.75261200	1.65718900
C	0.38358300	3.04052700	1.81304500
C	2.08289300	3.54508800	-0.85700900

H	2. 11887200	3. 54923600	-1. 95274500
H	3. 02815600	3. 95909300	-0. 51084900
N	2. 08271800	2. 16955200	-0. 36556800
C	3. 24917200	1. 54488500	0. 02165500
N	3. 08784300	0. 22061300	0. 32134900
C	4. 06634000	-0. 70643600	0. 76369300
C	5. 03481200	-0. 39992600	1. 72961500
C	3. 99826500	-2. 00679000	0. 25449200
C	5. 93714600	-1. 37968300	2. 13962500
C	4. 90253100	-2. 97938000	0. 68426100
H	3. 22803100	-2. 26085800	-0. 46261800
C	5. 88678600	-2. 67483400	1. 61981600
H	6. 59549400	-3. 42725600	1. 94288300
C	4. 80641600	-4. 35504800	0. 08429800
C	6. 93603000	-1. 06199000	3. 22096100
F	5. 14753100	-4. 35022000	-1. 23675700
F	5. 62019800	-5. 24223400	0. 69160500
F	3. 54886900	-4. 84362700	0. 14604900
F	8. 08781800	-1. 75223000	3. 05504500
F	7. 24954200	0. 24993000	3. 25619700
F	6. 46231500	-1. 38666200	4. 44798400
S	4. 72669000	2. 35641500	0. 15734400
C	1. 52172400	5. 97020100	-0. 67594500
H	0. 72796200	6. 68199400	-0. 43141800
H	1. 63568300	6. 02631500	-1. 76247900
H	5. 08900800	0. 59420000	2. 14789900
C	-0. 88825300	2. 45619300	1. 89074200
H	2. 18819800	-0. 22588800	0. 12531100
O	0. 94115100	-1. 71055600	0. 17415000
H	1. 29584600	1. 57406300	-0. 61481900
O	0. 45116700	-1. 81024500	2. 64880000
H	-0. 76642900	1. 70015700	0. 78568900
C	-6. 36464200	-2. 72080700	0. 27828300
C	-5. 84986900	-2. 34831800	-0. 95711800
C	-4. 87384400	-1. 34234800	-1. 05971300
C	-4. 90771400	-1. 08507100	1. 36894700
C	-5. 91569800	-2. 06233700	1. 42044600
C	-2. 01096800	-0. 79505500	-2. 82097000
C	-3. 33681700	-0. 51972500	-3. 14898000
C	-3. 62020600	0. 14296400	-4. 35367400
C	-2. 61562300	0. 35812600	-5. 29202000
C	-1. 32903600	-0. 11272700	-5. 02358900
C	-0. 98476400	-0. 68552500	-3. 78552800
H	-6. 34177100	-2. 30565800	2. 38909400

H	-0.55967500	-0.03655900	-5.78571200
C	-4.64737100	-0.99696700	-2.52917800
C	-5.05271400	-2.36026800	-3.19491700
H	-4.19574300	-3.04169900	-3.14292100
H	-5.32303700	-2.24592100	-4.24856300
H	-5.59725600	-0.11423500	-5.21362500
H	-5.26426800	1.53354600	-4.69905100
C	-4.35532000	-0.78392800	0.10797000
H	-7.11845500	-3.50007700	0.35518200
H	-2.83243800	0.84207100	-6.24111900
C	-6.19739200	-2.90255700	-2.31917600
H	-6.25484600	-3.99685500	-2.32566400
H	-7.17462400	-2.53327500	-2.66091300
C	-5.09432200	0.48186700	-4.44015400
C	-5.61151500	0.12942000	-3.02569500
H	-5.51191300	0.99664800	-2.36282300
H	-6.66032300	-0.18253700	-3.01414600
C	0.38557000	-1.24795200	-3.57493600
C	1.53598700	-0.42611300	-3.69320000
C	0.53253400	-2.64136700	-3.34177700
C	1.47908800	0.96958700	-4.01336400
C	2.84859400	-1.00217500	-3.49832100
C	1.84933900	-3.19512200	-3.12439800
C	2.61674500	1.72555000	-4.14496400
H	0.51350900	1.43168800	-4.17670700
C	4.00760600	-0.17306300	-3.61865800
C	2.96817400	-2.36131000	-3.19794800
C	3.90300900	1.15327800	-3.93792200
H	2.53512700	2.77641300	-4.41095500
H	4.98111300	-0.62674500	-3.45134300
H	3.95492800	-2.78286500	-3.02290600
H	4.79152100	1.77098400	-4.02626600
C	-4.57416800	-0.37160000	2.64308200
C	-3.93712600	-1.06113300	3.70316300
C	-5.04913400	0.95077300	2.83436400
C	-3.42082000	-2.38922400	3.56365900
C	-3.78008200	-0.41037600	4.98520000
C	-4.86200500	1.59713300	4.11421600
C	-2.81844100	-3.03072600	4.61360800
H	-3.47918000	-2.87446400	2.59763800
C	-3.15343300	-1.12006300	6.05707600
C	-4.24128900	0.89786900	5.15317400
C	-2.69014600	-2.39519800	5.88120000
H	-2.41324400	-4.02800700	4.47238700

H	-3.04987300	-0.61747300	7.01589400
H	-4.11925200	1.38299100	6.11978200
H	-2.20983600	-2.92281400	6.70059900
C	-0.38530200	-4.89810600	-3.12880800
H	-1.24062700	-5.56819800	-3.15315100
C	-0.56644800	-3.55893400	-3.35483100
H	-1.56128900	-3.18682500	-3.56954400
C	0.90813000	-5.42480500	-2.85695800
H	1.02824600	-6.48605000	-2.65792900
C	1.99426500	-4.59343400	-2.85897800
H	2.99006600	-4.97559500	-2.65599600
C	-6.18949600	2.96355800	2.03805900
H	-6.71498300	3.49432700	1.24860200
C	-5.97764700	3.60419000	3.29189200
H	-6.33677400	4.61794900	3.44716600
C	-5.33605600	2.93405500	4.29856300
H	-5.18113600	3.40427200	5.26703400
C	-5.74493900	1.68520500	1.81954300
H	-5.92726900	1.21154200	0.86150500
C	-0.34275000	4.40349600	-1.21458400
C	-1.34737500	5.38300900	-1.08603400
C	-0.56128100	3.38854700	-2.15171500
C	-2.50346600	5.35357500	-1.86224800
H	-1.23850600	6.18673600	-0.36316900
C	-1.72128600	3.34836900	-2.93097300
H	0.17111800	2.60396300	-2.28870400
C	-2.69519000	4.33347800	-2.79585000
H	-3.25381100	6.12971100	-1.73558700
H	-1.85854300	2.53824300	-3.64086600
H	-3.59471200	4.30735600	-3.40513900
C	2.78960400	6.44009900	0.01909100
C	4.01106900	6.40991300	-0.55920500
C	2.59613500	7.05955000	1.40130300
H	1.53375000	7.15959600	1.64474200
H	3.05740600	6.47023600	2.20474100
H	3.02933800	8.06484300	1.45959900
C	1.51855700	2.43196800	2.58587500
H	1.53929000	1.34090700	2.52875100
H	2.49049400	2.82522000	2.28590500
H	1.35978000	2.67701700	3.64870800
C	-1.13670600	1.39655900	2.97152900
H	-0.38563400	0.60674400	3.01480900
H	-1.18068300	1.88078100	3.95618200
H	-2.09835900	0.91293500	2.80143200

C	5.25730500	6.89700500	0.14549300
H	6.02260200	6.10957600	0.13760700
H	5.69093400	7.75816800	-0.38305000
H	5.09308600	7.18699200	1.18440900
C	4.30978700	5.88908600	-1.94664700
H	4.83897800	4.92816900	-1.88719100
H	3.42432800	5.74113700	-2.56851900
H	4.97408000	6.58642400	-2.47417700
C	-2.15483000	3.25133900	1.56803500
H	-2.01379100	3.99793500	0.79047000
H	-2.94830200	2.57651800	1.23949100
H	-2.51181500	3.74838100	2.47996700

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l imaginary frequency

H = -5472.468087

G = -5472.679258

E(M06-2X-DCM) = -5473.451356

O	1.55423300	-0.79387800	1.86638300
O	3.25023500	-0.05191200	0.01958100
P	1.69202200	-0.43268600	0.28665100
O	0.90348100	0.83747200	-0.07598200
N	1.38829400	-1.78283200	-0.51374800
S	-0.09641600	-2.36289100	-0.62738600
C	0.07832800	-4.06292700	0.12714800
F	0.56856200	-3.97217600	1.36411500
F	0.90319400	-4.81845700	-0.61086200
F	-1.12302700	-4.64325500	0.16722100
C	-0.78798200	4.38344500	-1.25435200
C	-0.45787400	3.73079800	-2.66275800
H	0.39896400	4.27923900	-3.06854400
H	-1.31352600	3.95322400	-3.30791200
C	-0.19381500	2.24724300	-2.83270400
C	-1.95093600	3.64851800	-0.53013400
H	-1.98796800	3.98197200	0.51130900
H	-2.88561600	3.97108300	-0.98522400
N	-2.00232100	2.18912100	-0.58450100
C	-3.18005300	1.51857200	-0.84054400
N	-3.08821800	0.16683700	-0.66203200
C	-4.09431600	-0.81804300	-0.83542400
C	-4.99232600	-0.82524300	-1.91166700
C	-4.12703300	-1.86775800	0.08768100
C	-5.92596200	-1.85375000	-2.02562100
C	-5.06140600	-2.89559400	-0.04710600

H	-3.41088100	-1.88811300	0.89946300
C	-5.97660900	-2.89424200	-1.09549500
H	-6.70967600	-3.68554500	-1.19167800
C	-5.07275500	-3.98558600	0.98899300
C	-6.84846300	-1.88987000	-3.21560000
F	-5.45800300	-3.51191800	2.20899600
F	-5.91869700	-4.98787600	0.67654600
F	-3.84673000	-4.52430600	1.16516100
F	-8.04757900	-2.43180100	-2.90082100
F	-7.07788700	-0.66010500	-3.72088200
F	-6.33563900	-2.63957200	-4.22066200
S	-4.58384200	2.29539300	-1.37612100
C	-1.36611700	5.82093200	-1.60397000
H	-2.10650700	5.66776600	-2.39077800
H	-0.56091900	6.41087100	-2.05837300
H	-4.96907100	-0.03226200	-2.64426700
C	1.04969300	1.62937400	-2.63899600
H	-2.23195000	-0.22113400	-0.25743700
O	-1.05917800	-1.66825100	0.26625400
H	-1.27334100	1.67400200	-0.09533600
O	-0.50269600	-2.58869200	-2.01782100
H	0.84702400	1.28161600	-1.35599900
C	6.17668500	-2.94067200	0.86495500
C	5.63981600	-2.15695200	1.87867700
C	4.71808600	-1.13579500	1.59110300
C	4.85301700	-1.70442100	-0.78049400
C	5.80645600	-2.68281400	-0.45272200
C	1.83079400	0.08282800	2.91829600
C	3.15689100	0.39972700	3.20455600
C	3.43264000	1.41896300	4.12965900
C	2.40728000	1.98082200	4.88411400
C	1.10683800	1.50025300	4.72023300
C	0.77681800	0.55546400	3.73125100
H	6.25314800	-3.25184200	-1.26247100
H	0.31527700	1.86263800	5.36875400
C	4.45995100	-0.31040200	2.84885300
C	4.76519000	-1.38773300	3.94955200
H	3.87386600	-2.01154600	4.08313700
H	5.00482000	-0.93875400	4.91773300
H	5.35866800	1.38379900	5.13089500
H	5.13996400	2.77533700	4.07901000
C	4.27297500	-0.97878400	0.27905800
H	6.88830700	-3.73086800	1.08988800
H	2.61548300	2.74891100	5.62481800

C	5.90761500	-2.23821100	3.36363900
H	5.90318300	-3.26886400	3.73586600
H	6.89148700	-1.81672200	3.61357900
C	4.91951600	1.70590100	4.17699000
C	5.46720800	0.87714800	2.99136100
H	5.44113900	1.47416100	2.07247800
H	6.49652200	0.53705600	3.14060900
C	-0.61478800	0.01285800	3.64566300
C	-1.71948200	0.87476800	3.42173400
C	-0.83329400	-1.37109600	3.87960700
C	-1.59436300	2.29368800	3.26277100
C	-3.05511100	0.32223300	3.35879900
C	-2.17070300	-1.90997800	3.78577500
C	-2.69129200	3.09750700	3.07844500
H	-0.61023200	2.74304500	3.31169600
C	-4.16853200	1.19191000	3.13691200
C	-3.24157500	-1.05309200	3.51865700
C	-3.99991800	2.54333300	3.00569800
H	-2.56013100	4.17245800	2.98427000
H	-5.15970400	0.74953500	3.07795700
H	-4.24390000	-1.46707300	3.44008300
H	-4.85438700	3.19212700	2.83885500
C	4.60583200	-1.44116000	-2.23415700
C	3.97108900	-2.41707300	-3.04013800
C	5.15818500	-0.27607700	-2.82454200
C	3.37875800	-3.60283700	-2.49887200
C	3.89595600	-2.22153700	-4.47118600
C	5.05290700	-0.08297000	-4.25367000
C	2.78111200	-4.53159000	-3.30946200
H	3.37576900	-3.74303300	-1.42533800
C	3.27110700	-3.22082100	-5.28127000
C	4.43316400	-1.06175000	-5.03571800
C	2.73354000	-4.34687300	-4.72041000
H	2.31791400	-5.40945800	-2.86957800
H	3.22973000	-3.06011900	-6.35602700
H	4.37260700	-0.91943600	-6.11304500
H	2.25555100	-5.09674900	-5.34466100
C	-0.04010700	-3.60668400	4.47452300
H	0.77356600	-4.26572300	4.76570100
C	0.20935800	-2.27735100	4.25562300
H	1.21516600	-1.89724600	4.39015100
C	-1.35051500	-4.13918000	4.32110800
H	-1.52405000	-5.20024000	4.47697600
C	-2.38610700	-3.30957600	3.98927700

H	-3.39392800	-3.69536300	3.86941700
C	6.37591700	1.84079100	-2.67635500
H	6.90026800	2.58206600	-2.07913700
C	6.24488900	2.03793900	-4.08039800
H	6.66371900	2.92828000	-4.54153400
C	5.60496500	1.09790800	-4.84258800
H	5.51091800	1.22662600	-5.91850900
C	5.85518100	0.72530700	-2.07297300
H	5.97686500	0.58893100	-1.00430600
C	0.49467000	4.53202400	-0.41490500
C	1.52300900	5.39627800	-0.83856800
C	0.69056600	3.85213700	0.79142100
C	2.67848500	5.58469400	-0.08436900
H	1.42823200	5.93831600	-1.77551200
C	1.84948700	4.03210800	1.55309100
H	-0.05970700	3.16512400	1.16007100
C	2.84584400	4.90419800	1.12351500
H	3.44737500	6.26489500	-0.44159800
H	1.96710900	3.48155000	2.48169300
H	3.74461600	5.05022100	1.71670000
C	-1.98370300	6.63260600	-0.47211500
C	-3.31686800	6.84438600	-0.37327900
C	-0.98739700	7.24441200	0.49629300
H	-0.59429600	6.51195300	1.21231400
H	-0.11703300	7.63038900	-0.04723200
H	-1.40638700	8.07547500	1.06596500
C	-1.31756800	1.45641700	-3.43818600
H	-1.39134900	0.44232800	-3.03782400
H	-2.28355800	1.95248700	-3.33860200
H	-1.09669200	1.34309600	-4.51212800
C	1.29248000	0.26515000	-3.29733000
H	0.50834300	-0.47177800	-3.11854000
H	1.39864200	0.39474000	-4.38261600
H	2.22333000	-0.16327500	-2.92630900
C	-3.95964700	7.62911500	0.75300900
H	-4.36531300	8.58191800	0.38308300
H	-4.81505400	7.06839100	1.15304500
H	-3.29418400	7.84775900	1.58901800
C	-4.36359600	6.33765500	-1.34380000
H	-5.09449600	7.13181600	-1.54672400
H	-3.97141900	6.00214100	-2.30541000
H	-4.92340400	5.49532300	-0.91558000
C	2.34041400	2.44300000	-2.52274700
H	2.20234500	3.41489400	-2.05586400

H	3.07930900	1.89376600	-1.93488100
H	2.76759100	2.58567500	-3.52438200

TS-1-2-7SR-2

l imaginary frequency

H = -5472.467373

G = -5472.678369

E(M06-2X-DCM) = -5473.451709

O	-1.62171900	-1.59537800	-1.34135000
O	-3.22009000	-0.04760000	0.03584300
P	-1.67686300	-0.54034600	-0.10465900
O	-0.87667400	0.73841100	-0.41229300
N	-1.32561400	-1.36987300	1.21536700
S	0.15857400	-1.88610500	1.50845600
C	-0.07117900	-3.73782000	1.60142500
F	-0.63671400	-4.19144900	0.48181000
F	-0.85372800	-4.05923500	2.64140200
F	1.12163800	-4.31504400	1.76141900
C	0.74699400	4.41558900	-1.13090300
C	0.50925700	4.50760800	0.42487600
H	-0.36567700	5.14722400	0.57690600
H	1.37727900	5.04382200	0.82083500
C	0.34634100	3.27222100	1.28479500
C	1.92130000	3.46243900	-1.47934300
H	1.96043600	3.33283400	-2.56811000
H	2.84804400	3.95206300	-1.19314400
N	1.98891200	2.16175000	-0.81655500
C	3.18775300	1.64190400	-0.37826100
N	3.09073200	0.36892800	0.11077000
C	4.11905300	-0.43628300	0.66690400
C	5.07013600	0.05380100	1.57234100
C	4.12005400	-1.79649700	0.34568200
C	6.02327800	-0.80924200	2.10946400
C	5.07359900	-2.65053600	0.90271800
H	3.36453100	-2.18902100	-0.32276700
C	6.04036300	-2.16593700	1.77842200
H	6.78732400	-2.82738700	2.19950200
C	5.04506200	-4.10179700	0.50933400
C	7.00465400	-0.29043500	3.12707200
F	5.36163600	-4.27068700	-0.80691500
F	5.91827100	-4.84680300	1.21696400
F	3.81842300	-4.64247800	0.67346000
F	8.19200000	-0.93432900	3.04896400
F	7.24646700	1.02849600	2.97618600

F	6.55083700	-0.46528500	4.39154200
S	4.63426000	2.51841700	-0.40180300
C	1.19561600	5.86095800	-1.62973900
H	0.36157100	6.53812600	-1.44400400
H	1.26989200	5.78606300	-2.72179300
H	5.07163400	1.09853000	1.84608100
C	-0.87396500	2.61902400	1.50613400
H	2.20951700	-0.13980000	0.00540200
O	1.07452900	-1.69300900	0.35559300
H	1.21682200	1.51247600	-0.95134500
O	0.63524700	-1.48331500	2.83433100
H	-0.74922800	1.71475200	0.51222900
C	-6.15840500	-2.94163400	0.82285200
C	-5.69180400	-2.73674300	-0.46947700
C	-4.76620500	-1.71714800	-0.75029500
C	-4.75194700	-1.10162400	1.61331000
C	-5.71236300	-2.10157200	1.84017700
C	-1.97568000	-1.31874900	-2.66422500
C	-3.32112600	-1.15188500	-2.98623900
C	-3.66612900	-0.69100400	-4.26669800
C	-2.69785800	-0.57858700	-5.25945600
C	-1.38434500	-0.94927800	-4.96592400
C	-0.98168500	-1.31353200	-3.66805500
H	-6.10251800	-2.21533200	2.84707800
H	-0.63932100	-0.95720600	-5.75553400
C	-4.59210400	-1.58623100	-2.26100600
C	-4.94944300	-3.04975600	-2.70421000
H	-4.06068200	-3.67879500	-2.57821000
H	-5.25018900	-3.10587800	-3.75430800
H	-5.65032100	-1.15700300	-5.01507900
H	-5.38106600	0.56172700	-4.76190100
C	-4.24559800	-0.96901500	0.30483300
H	-6.87317700	-3.73172700	1.03793600
H	-2.96189500	-0.25338700	-6.26272700
C	-6.04612600	-3.50285100	-1.72274000
H	-6.05276400	-4.58721700	-1.56486600
H	-7.04745800	-3.23061500	-2.08517200
C	-5.15608100	-0.43121500	-4.35518100
C	-5.62021200	-0.58908000	-2.88830100
H	-5.54474300	0.37120600	-2.36529300
H	-6.65259300	-0.94019000	-2.79692400
C	0.41842700	-1.78128700	-3.42366600
C	1.52583000	-0.93745100	-3.69617200
C	0.63588700	-3.11916900	-2.99932000

C	1. 39548700	0. 39358700	-4. 21066600
C	2. 86848500	-1. 42328200	-3. 46436900
C	1. 98245800	-3. 58043200	-2. 75054700
C	2. 49251800	1. 17207900	-4. 48172200
H	0. 40535900	0. 78348400	-4. 41090300
C	3. 98381500	-0. 57034500	-3. 73609300
C	3. 05903800	-2. 71951600	-2. 97936700
C	3. 80899000	0. 69188700	-4. 23438700
H	2. 35496400	2. 16946800	-4. 89169500
H	4. 98143400	-0. 95314500	-3. 53668600
H	4. 06859200	-3. 06957000	-2. 77893500
H	4. 66479700	1. 32937500	-4. 43425100
C	-4. 41994800	-0. 19420200	2. 75801500
C	-3. 72525900	-0. 69207500	3. 88705400
C	-4. 95201500	1. 12011200	2. 76905700
C	-3. 15179900	-2. 00327400	3. 92751800
C	-3. 56593100	0. 14723500	5. 05412700
C	-4. 76292200	1. 95587500	3. 93380200
C	-2. 49218900	-2. 45588100	5. 03959900
H	-3. 21316900	-2. 62860900	3. 04601600
C	-2. 87900900	-0. 36872800	6. 19743800
C	-4. 08340100	1. 44512400	5. 04332100
C	-2. 36070400	-1. 63480300	6. 19530500
H	-2. 04399300	-3. 44469500	5. 03245000
H	-2. 77442400	0. 27411500	7. 06834400
H	-3. 95938600	2. 07263700	5. 92390000
H	-1. 83457800	-2. 01421300	7. 06692700
C	-0. 17057400	-5. 35803700	-2. 43624900
H	-0. 99440300	-6. 05968900	-2. 33541100
C	-0. 41963100	-4. 07388900	-2. 84396500
H	-1. 43622200	-3. 77786400	-3. 07465700
C	1. 15289300	-5. 78580600	-2. 13667200
H	1. 32733000	-6. 80146800	-1. 79276100
C	2. 19902500	-4. 91874700	-2. 29380600
H	3. 21660200	-5. 22576700	-2. 07197300
C	-6. 20767900	2. 94169400	1. 72455300
H	-6. 77835300	3. 32666700	0. 88358100
C	-5. 99422700	3. 76908600	2. 86353800
H	-6. 39732100	4. 77806200	2. 88050300
C	-5. 29532000	3. 28352500	3. 93585900
H	-5. 13799400	3. 89786800	4. 81953300
C	-5. 70830500	1. 66568800	1. 68100600
H	-5. 89255400	1. 04835400	0. 80898000
C	-0. 55865900	4. 10971500	-1. 89384800

C	-1.63255700	5.02119500	-1.86185600
C	-0.71598700	2.97064700	-2.68979300
C	-2.79728800	4.80804500	-2.59512600
H	-1.57203700	5.91708500	-1.25025400
C	-1.88367000	2.74632600	-3.42495800
H	0.07270800	2.23225000	-2.74931500
C	-2.92769700	3.66588200	-3.38711800
H	-3.60226500	5.53675500	-2.54601900
H	-1.97174200	1.84491500	-4.02378000
H	-3.83373500	3.49595600	-3.96266100
C	2.48231400	6.47676000	-1.09911600
C	2.51497900	7.34243800	-0.06012500
C	3.75309400	6.15408400	-1.87822400
H	4.43075800	5.48439200	-1.33419200
H	3.51624300	5.65937100	-2.82492800
H	4.31540200	7.06199600	-2.12291800
C	1.55273100	2.87387700	2.08462600
H	1.65019400	1.79216100	2.20288800
H	2.48042100	3.27561400	1.67529900
H	1.42029000	3.28097000	3.10039000
C	-1.00471100	1.71648800	2.73923000
H	-0.19671100	0.99330800	2.85979000
H	-1.04685500	2.33530400	3.64550900
H	-1.93344500	1.14849900	2.68700700
C	3.80538100	7.96258900	0.43323400
H	3.88595700	9.01080700	0.10842600
H	3.82805100	7.97743100	1.53063000
H	4.69818600	7.43606800	0.09214800
C	1.31088100	7.84266400	0.70723600
H	1.33055500	8.94026500	0.75619700
H	0.35081200	7.54977000	0.27790500
H	1.32945800	7.49123200	1.74857900
C	-2.20504600	3.27226800	1.12716800
H	-2.14945900	3.87999900	0.22723700
H	-2.96537900	2.50646100	0.96146000
H	-2.55337000	3.89793500	1.95988000

TS-1-2-7SR-3

l imaginary frequency

H = -5472.465895

G = -5472.677387

E(M06-2X-DCM) = -5473.447303

0	1.33425600	-1.28551400	1.82081000
0	3.13859000	-0.68588200	0.03013400

P	1.53736600	-0.80955600	0.28035700
O	0.99030600	0.60915500	0.04923300
N	0.99240400	-2.00156800	-0.63574600
S	-0.57461500	-2.24762600	-0.82314100
C	-0.76837200	-4.02289800	-0.27515500
F	-0.31463300	-4.17415800	0.96929000
F	-0.08628100	-4.83902200	-1.08870400
F	-2.06272400	-4.34670400	-0.31855100
C	-0.17886100	4.46416700	-0.85094900
C	0.00578900	3.83486500	-2.29752100
H	0.89808000	4.31247900	-2.71818900
H	-0.85220700	4.18521500	-2.88035400
C	0.11591500	2.34801000	-2.57476300
C	-1.35578700	3.79073300	-0.06891000
H	-1.18032400	3.88077300	1.00346900
H	-2.26826000	4.34087900	-0.28863000
N	-1.69221000	2.39894900	-0.36149300
C	-2.97750200	2.02550700	-0.70317300
N	-3.17681700	0.67570400	-0.64079900
C	-4.35686700	-0.07420000	-0.86542100
C	-5.30456200	0.22393700	-1.85448700
C	-4.53335300	-1.21602500	-0.07418700
C	-6.42203400	-0.59592800	-2.00852300
C	-5.65500000	-2.02646700	-0.24555300
H	-3.78593500	-1.47448800	0.66609800
C	-6.61616800	-1.72113700	-1.20556300
H	-7.49284200	-2.34454700	-1.33002700
C	-5.82216900	-3.21046900	0.66681400
C	-7.40345300	-0.30600800	-3.11415000
F	-6.09991600	-2.82019300	1.94435800
F	-6.82728600	-4.02212900	0.28164700
F	-4.69757100	-3.95496000	0.73764300
F	-8.65878800	-0.68311700	-2.77883800
F	-7.44317000	1.00484800	-3.42974400
F	-7.08629300	-0.97531900	-4.24831900
S	-4.15084400	3.13797200	-1.19656100
C	-0.61244600	5.96079700	-1.17986400
H	-1.65430400	5.90117600	-1.52557900
H	-0.03628500	6.27876400	-2.04894700
H	-5.17747100	1.09092400	-2.48518700
C	1.28905100	1.59655400	-2.42751400
H	-2.41712400	0.09399000	-0.27655600
O	-1.40556600	-1.47782600	0.14070300
H	-1.11424200	1.68996900	0.08535600

O	-0.98345000	-2.22102500	-2.23186700
H	1.01314000	1.16281700	-1.17976400
C	5.55166200	-4.06262300	0.65781500
C	5.13952900	-3.27739000	1.72740100
C	4.39679700	-2.10298600	1.51757000
C	4.46084900	-2.51269800	-0.88961900
C	5.24041400	-3.65374600	-0.63678400
C	1.73307300	-0.53862400	2.93306000
C	3.08906200	-0.45608500	3.23903700
C	3.51350400	0.44441200	4.22848000
C	2.58121100	1.11382200	5.01567300
C	1.22295200	0.85806100	4.82018200
C	0.75744200	0.04364800	3.77113900
H	5.59811100	-4.22652700	-1.48708900
H	0.49267400	1.30090700	5.49007400
C	4.26501000	-1.33845400	2.83224600
C	4.38518100	-2.52618900	3.85209800
H	3.40414500	-3.00605800	3.94559500
H	4.68764500	-2.19139500	4.84853000
H	5.39654100	0.02989500	5.22554300
H	5.41816700	1.50743400	4.27292800
C	3.99401200	-1.78293600	0.22145500
H	6.12479900	-4.97129800	0.82284900
H	2.90007000	1.79051100	5.80450400
C	5.37960100	-3.50611900	3.20177200
H	5.20631100	-4.54633900	3.49968000
H	6.41676900	-3.26790200	3.47675300
C	5.02660100	0.48380200	4.29617000
C	5.44762800	-0.33994700	3.05626100
H	5.52795800	0.31453800	2.18064000
H	6.40756800	-0.85004700	3.18191300
C	-0.70153300	-0.25709200	3.63729500
C	-1.64883600	0.78987600	3.49217300
C	-1.14573500	-1.60261300	3.74353100
C	-1.29361300	2.17847400	3.46006000
C	-3.05603000	0.46961500	3.38597100
C	-2.55019100	-1.90663900	3.59245600
C	-2.24678900	3.16245800	3.37774100
H	-0.24849600	2.45715700	3.52202000
C	-4.01338200	1.52510600	3.26534100
C	-3.46438100	-0.86620100	3.40930700
C	-3.62820400	2.83786300	3.27286000
H	-1.94340300	4.20615700	3.38673500
H	-5.06273700	1.25630400	3.17456300

H	-4. 51937600	-1. 10278300	3. 29356300
H	-4. 36601000	3. 63005600	3. 18839100
C	4. 27642700	-2. 10218400	-2. 31811300
C	3. 49733200	-2. 89383000	-3. 19579400
C	5. 01750100	-1. 00036700	-2. 81630200
C	2. 71316200	-4. 00473000	-2. 74744200
C	3. 46955400	-2. 57763200	-4. 60674700
C	4. 96029000	-0. 68228300	-4. 22562400
C	1. 98091700	-4. 75783600	-3. 62700700
H	2. 67774100	-4. 22645600	-1. 68810400
C	2. 69749100	-3. 39455800	-5. 49092300
C	4. 19633800	-1. 48216600	-5. 08021700
C	1. 97802800	-4. 45806600	-5. 01891100
H	1. 37801900	-5. 58146500	-3. 25696700
H	2. 69341800	-3. 14577900	-6. 54955600
H	4. 17083700	-1. 24850300	-6. 14289400
H	1. 39070600	-5. 06893200	-5. 69888900
C	-0. 73663500	-3. 98244900	4. 13282400
H	-0. 04652600	-4. 78832000	4. 36846400
C	-0. 27183000	-2. 69672000	4. 04213400
H	0. 77837900	-2. 49898900	4. 22136200
C	-2. 11142800	-4. 27936500	3. 91814300
H	-2. 45662100	-5. 30810600	3. 97116900
C	-2. 99244100	-3. 26559900	3. 65958600
H	-4. 04661500	-3. 46973200	3. 49770900
C	6. 55767100	0. 87476800	-2. 50457000
H	7. 18682000	1. 47398700	-1. 85175300
C	6. 47666000	1. 19800700	-3. 88885200
H	7. 03831800	2. 04226600	-4. 27935300
C	5. 70263700	0. 43529200	-4. 72138100
H	5. 64225100	0. 66062500	-5. 78371500
C	5. 85757200	-0. 18550300	-1. 98954000
H	5. 94349000	-0. 42162900	-0. 93490900
C	1. 14793800	4. 46003600	-0. 07182400
C	2. 17987700	5. 34527100	-0. 43612600
C	1. 39587400	3. 59467400	1. 00115500
C	3. 39678700	5. 36680700	0. 24188400
H	2. 04060900	6. 02732400	-1. 26789300
C	2. 61576700	3. 60895700	1. 68424900
H	0. 65099600	2. 87276900	1. 31023000
C	3. 62035300	4. 49843400	1. 31227200
H	4. 17007100	6. 06580000	-0. 06656100
H	2. 77246300	2. 91382700	2. 50439100
H	4. 56805500	4. 51456100	1. 84402400

C	-0.51735600	7.02172600	-0.09319800
C	0.15259300	8.18449400	-0.26220000
C	-1.29737300	6.71174700	1.16839000
H	-2.28277000	6.29982600	0.92066900
H	-0.78265900	5.96216100	1.78456800
H	-1.46687200	7.58802100	1.79489600
C	-1.07136700	1.72345600	-3.25141000
H	-1.26329400	0.69815400	-2.92418500
H	-1.97901100	2.31580100	-3.13420000
H	-0.83969000	1.65727900	-4.32677800
C	1.40578200	0.27513900	-3.19648500
H	0.53992300	-0.38129100	-3.10508300
H	1.56417400	0.48621200	-4.26248800
H	2.27255400	-0.28251200	-2.84231700
C	0.26053600	9.26054700	0.79956800
H	1.30766800	9.57559400	0.90462700
H	-0.30211200	10.15864800	0.50625900
H	-0.08442900	8.95564000	1.78777100
C	0.88901200	8.60188900	-1.51863000
H	1.97036200	8.66785700	-1.33018500
H	0.73919100	7.95021400	-2.38087800
H	0.57047300	9.60955800	-1.81882100
C	2.65371300	2.25843200	-2.22732300
H	2.60725400	3.21164200	-1.70661300
H	3.31288700	1.59698900	-1.65941900
H	3.12268700	2.41240000	-3.20860200

TS-1-2-7RS

l imaginary frequency

H = -5472.459963

G = -5472.673821

E(M06-2X-DCM) = -5473.441135

O	-1.94453500	1.27887300	1.49966300
O	-3.29286400	-0.82300600	0.71373600
P	-1.97874800	0.07904500	0.39180700
O	-2.09836300	0.78675800	-0.95225700
N	-0.68054700	-0.82498500	0.67702400
S	-0.45796700	-2.33340900	0.20894200
C	-0.85399900	-3.35204100	1.73033600
F	-0.75796200	-4.64725000	1.42718400
F	0.01000900	-3.07394900	2.71688800
F	-2.09273200	-3.09122400	2.15982000
C	1.46084600	3.08841900	-2.44742200
C	1.18075000	1.96857200	-3.54633900

H	0.70387500	2.49726900	-4.38087400
H	2.16790000	1.64324000	-3.88493500
C	0.38664900	0.69425400	-3.31475100
C	2.22690300	2.53093100	-1.19251600
H	1.84990500	3.01407100	-0.29023300
H	3.27025100	2.82710900	-1.28893200
N	2.24209700	1.08853500	-0.94355600
C	3.37340200	0.32774700	-1.11947700
N	3.28827300	-0.91577700	-0.55926500
C	4.31391700	-1.88341000	-0.45113400
C	5.61423200	-1.54053400	-0.06591300
C	3.98512200	-3.23178600	-0.63756100
C	6.56578800	-2.53941700	0.13233700
C	4.95307400	-4.21873600	-0.44592500
H	2.97154700	-3.50608300	-0.90521600
C	6.25049500	-3.88408200	-0.05968400
H	6.99491600	-4.65380100	0.10119000
C	4.60370200	-5.65801100	-0.71863400
C	7.91321000	-2.13705400	0.66620200
F	3.31406200	-5.92840400	-0.42625200
F	5.37151900	-6.50647300	0.00221600
F	4.78637600	-5.97630400	-2.02200800
F	8.81951100	-3.13308600	0.58245800
F	7.83041600	-1.78604700	1.97825100
F	8.41789100	-1.06798400	0.01579100
S	4.69334700	0.85105000	-2.03534200
C	2.47506000	4.07023000	-3.17151300
H	3.23256500	3.42591200	-3.61564700
H	1.95737200	4.55178700	-4.01056200
H	5.87168300	-0.50324900	0.09644300
C	-1.01289500	0.59083600	-3.34358900
H	2.37549300	-1.24952200	-0.23946400
O	0.99138300	-2.55094100	0.01177300
H	1.57976400	0.74511000	-0.25278800
O	-1.36828300	-2.82269400	-0.83334000
H	-1.29718600	0.69856100	-2.03477300
C	-7.11433900	0.90638200	0.58854900
C	-6.26924800	1.12128600	1.67146400
C	-5.03429000	0.46126100	1.74882800
C	-5.45127700	-0.59948200	-0.40884600
C	-6.71869000	0.01544300	-0.40638900
C	-1.85727100	0.96385900	2.86886200
C	-3.00211000	0.53289500	3.54086700
C	-2.88612400	0.05130300	4.85559100

C	-1.67210700	0.10378300	5.52835400
C	-0.57568900	0.67280300	4.88714500
C	-0.63309500	1.11229600	3.55225700
H	-7.39758300	-0.21344000	-1.22169700
H	0.36464900	0.78014700	5.41870400
C	-4.47719900	0.59676100	3.15876100
C	-5.10680400	1.96796200	3.57700000
H	-5.15555900	2.09157700	4.66306000
H	-4.48456800	2.77713600	3.17701000
H	-4.11434300	-1.44872900	5.85199900
H	-4.65774700	0.20806600	6.09277000
C	-4.59371600	-0.30102000	0.66924800
H	-8.08333000	1.39558900	0.52987900
H	-1.58126300	-0.26581100	6.54644000
C	-6.49199700	1.98480300	2.89406400
H	-7.26693000	1.55877400	3.54614000
H	-6.82305100	2.99752600	2.63643300
C	-4.21135300	-0.47568000	5.35725600
C	-5.05095400	-0.54420400	4.06688800
H	-6.12662700	-0.44046400	4.23739200
H	-4.88246800	-1.50532600	3.56757100
C	0.58120200	1.80982100	3.02172000
C	0.54336700	3.21627200	2.83510500
C	1.81264400	1.11397600	2.92759600
C	-0.64738500	3.99597000	2.99949100
C	1.76318400	3.92664700	2.51920100
C	3.03098000	1.84555000	2.65936900
C	-0.64407000	5.35549500	2.82425000
H	-1.56685400	3.49614200	3.28155000
C	1.72008400	5.34427700	2.33057600
C	2.97066600	3.22534200	2.44676000
C	0.55177300	6.04278900	2.47310300
H	-1.56344600	5.91892100	2.95926000
H	2.64660800	5.85679600	2.08331900
H	3.88898700	3.77067900	2.23932800
H	0.53368400	7.11980700	2.33222800
C	-5.13847700	-1.57455900	-1.49742500
C	-4.87978700	-2.93442100	-1.18274800
C	-5.23249800	-1.16535200	-2.85354300
C	-4.84298200	-3.43767800	0.15682700
C	-4.67956200	-3.88759500	-2.25089800
C	-5.07722000	-2.14266600	-3.90813000
C	-4.57742400	-4.75538100	0.42117000
H	-5.03647800	-2.76157600	0.98027900

C	-4.39770400	-5.25286200	-1.93326600
C	-4.79333600	-3.46981600	-3.57858700
C	-4.33894700	-5.67851000	-0.63507600
H	-4.54923100	-5.10214800	1.45054100
H	-4.23464700	-5.94715400	-2.75399500
H	-4.66311000	-4.19822400	-4.37638000
H	-4.12104000	-6.71767500	-0.40501400
C	3.13330600	-0.93576900	3.08754700
H	3.17964500	-2.01248100	3.22396900
C	1.91707600	-0.30345400	3.11047800
H	1.01258100	-0.87960900	3.25610100
C	4.33604900	-0.20351200	2.86958200
H	5.29066300	-0.72174800	2.85876000
C	4.27871000	1.14548900	2.64412600
H	5.18491600	1.71594000	2.45551400
C	-5.57461600	0.54859400	-4.56942500
H	-5.74758200	1.58841100	-4.83416400
C	-5.45794500	-0.42690600	-5.59964900
H	-5.55716100	-0.12884100	-6.63982400
C	-5.20634100	-1.73160500	-5.27218800
H	-5.09665300	-2.48694900	-6.04688800
C	-5.45982100	0.19444000	-3.24921900
H	-5.52893900	0.95853500	-2.48390800
C	0.14069100	3.80616100	-2.09227900
C	-0.43773300	4.72855600	-2.98762900
C	-0.56238200	3.54836100	-0.91004900
C	-1.63854000	5.37454800	-2.70324300
H	0.04782500	4.95220300	-3.93198800
C	-1.77424000	4.18365900	-0.62284100
H	-0.18606800	2.83866600	-0.18355200
C	-2.31570100	5.10649600	-1.51189700
H	-2.04580600	6.08559000	-3.41769300
H	-2.28528600	3.93914000	0.30210600
H	-3.25448600	5.60576500	-1.28741400
C	3.16643100	5.14607900	-2.33866900
C	4.51510800	5.25561100	-2.28181300
C	-1.62433500	-0.79331200	-3.60469400
H	-1.42699200	-1.09848900	-4.64188700
H	-1.25610700	-1.57511900	-2.93898000
H	-2.70423800	-0.74001700	-3.47381800
C	5.23917500	6.30708200	-1.46172300
H	5.65775700	7.09180300	-2.10879300
H	4.62374600	6.79237000	-0.70294300
H	6.09319500	5.84893700	-0.94586400

C	1.18475900	-0.57942000	-3.28524800
H	2.25769500	-0.40347300	-3.24213600
H	0.89359100	-1.24528700	-2.46679900
H	0.96239100	-1.13585100	-4.20851000
C	2.24744000	6.13977300	-1.65515200
H	1.49008400	6.50559200	-2.35804100
H	1.69167000	5.69579000	-0.81994700
H	2.77801600	7.01272900	-1.27298600
C	-1.88390800	1.71099300	-3.91572700
H	-2.87986000	1.67148500	-3.46929100
H	-1.48035300	2.70608000	-3.75182000
H	-2.00436100	1.54847500	-4.99584000
C	5.50818800	4.39173000	-3.03114800
H	6.07852300	3.76229500	-2.33606000
H	5.07191500	3.72954500	-3.77843300
H	6.23654800	5.03613700	-3.54344500

TS-1-2-7RS-1

l imaginary frequency

H = -5472.453344

G = -5472.668184

E(M06-2X-DCM) = -5473.435953

O	-2.06436300	1.00240100	1.62753200
O	-3.11442900	-1.15472500	0.57775500
P	-1.89916800	-0.08432500	0.41613800
O	-2.01949100	0.71651400	-0.87347300
N	-0.52137800	-0.85648400	0.69095500
S	-0.09749800	-2.35878000	0.40591400
C	-0.62451800	-3.32242900	1.92456400
F	-0.13818600	-4.56228800	1.84824200
F	-0.15603400	-2.73801600	3.03487500
F	-1.96068500	-3.38555000	2.00712900
C	1.30757900	3.11129200	-2.54065400
C	1.03675200	1.98491200	-3.63615300
H	0.45300800	2.47456400	-4.42420900
H	2.01848100	1.74874500	-4.05683500
C	0.37875400	0.64737000	-3.34080400
C	2.30999100	2.62738000	-1.44056700
H	2.16257200	3.22031100	-0.53488400
H	3.31379900	2.84201100	-1.79140900
N	2.34981500	1.21104700	-1.06980900
C	3.48240200	0.45111700	-1.25402800
N	3.45549400	-0.75063200	-0.60719600
C	4.52000200	-1.67914100	-0.49496200

C	5. 81796700	-1. 26850600	-0. 17096800
C	4. 23962500	-3. 04455000	-0. 61300400
C	6. 82009400	-2. 21700200	0. 02125600
C	5. 25523300	-3. 98329300	-0. 41999900
H	3. 22803500	-3. 36970300	-0. 82420100
C	6. 55215900	-3. 58030500	-0. 10630900
H	7. 33233600	-4. 31315800	0. 05822300
C	4. 95266100	-5. 44646200	-0. 61064400
C	8. 20626600	-1. 74177100	0. 36595500
F	3. 69378000	-5. 75437400	-0. 23453700
F	5. 79428300	-6. 23025700	0. 10062300
F	5. 07654400	-5. 81447800	-1. 90782700
F	8. 93795000	-2. 70704400	0. 96450700
F	8. 16874100	-0. 68131300	1. 21015400
F	8. 89256800	-1. 34410700	-0. 72731800
S	4. 74693100	0. 90952500	-2. 28216800
C	2. 05223000	4. 27606400	-3. 34949200
H	2. 57396600	3. 78944000	-4. 18072000
H	1. 29713800	4. 91536500	-3. 81110500
H	6. 03499600	-0. 21607900	-0. 05347700
C	-1. 00564600	0. 41211100	-3. 29101700
H	2. 58339000	-1. 07267300	-0. 17888900
O	1. 37816000	-2. 43045900	0. 46518200
H	1. 73403800	0. 91651000	-0. 31653400
O	-0. 77192500	-3. 01522900	-0. 72046800
H	-1. 25286100	0. 60233700	-1. 98790500
C	-7. 14285100	-0. 02694900	0. 97215000
C	-6. 26323100	0. 08124900	2. 04229700
C	-4. 93685300	-0. 36203100	1. 92565200
C	-5. 34589400	-0. 98101300	-0. 39982300
C	-6. 68652800	-0. 59001200	-0. 21532900
C	-1. 83389000	0. 56694200	2. 94761900
C	-2. 80584400	-0. 19687700	3. 59314300
C	-2. 49335900	-0. 82574200	4. 80996200
C	-1. 28142800	-0. 58261900	5. 44312200
C	-0. 39174200	0. 31721700	4. 86155100
C	-0. 63261700	0. 90210400	3. 60589300
H	-7. 37546500	-0. 73063200	-1. 04204100
H	0. 53194400	0. 56981000	5. 37304200
C	-4. 28970100	-0. 38908700	3. 30414100
C	-5. 11696500	0. 73164600	4. 02354400
H	-5. 08924200	0. 63640900	5. 11292300
H	-4. 68617300	1. 70557100	3. 76321500
H	-3. 27771600	-2. 71449000	5. 55967100

H	-4. 15154800	-1. 29624700	6. 12732300
C	-4. 46729100	-0. 80610900	0. 68931300
H	-8. 17654400	0. 29668200	1. 06334300
H	-1. 03792600	-1. 06140100	6. 38801000
C	-6. 53464700	0. 61433700	3. 43057000
H	-7. 15580300	-0. 08415200	4. 00847200
H	-7. 06932300	1. 57104900	3. 41616600
C	-3. 62780700	-1. 72030500	5. 25949200
C	-4. 53611100	-1. 76246100	4. 01248000
H	-5. 59200100	-1. 93024000	4. 24527400
H	-4. 20501200	-2. 56440700	3. 34377000
C	0. 35736800	1. 91413500	3. 12049400
C	-0. 00034200	3. 28721400	3. 12483900
C	1. 69555900	1. 53006200	2. 85540200
C	-1. 30191200	3. 75354300	3. 50226500
C	0. 99170200	4. 28492700	2. 79155500
C	2. 68931300	2. 54397500	2. 57534300
C	-1. 60993400	5. 08974400	3. 50994100
H	-2. 05078300	3. 02964800	3. 80276800
C	0. 62252100	5. 66687000	2. 79031900
C	2. 30505900	3. 88713200	2. 52348200
C	-0. 64131600	6. 06311800	3. 13519000
H	-2. 60371000	5. 41238500	3. 80903500
H	1. 38019000	6. 40005100	2. 52385400
H	3. 05467700	4. 64489000	2. 30450700
H	-0. 90599100	7. 11676300	3. 13817100
C	-4. 99586400	-1. 61369400	-1. 70899900
C	-4. 58007300	-2. 96952800	-1. 76129600
C	-5. 24389100	-0. 89888200	-2. 91118800
C	-4. 35380900	-3. 76625300	-0. 59364600
C	-4. 40640900	-3. 61196700	-3. 04558900
C	-5. 10468200	-1. 56955000	-4. 18460000
C	-3. 94544900	-5. 07038000	-0. 68508500
H	-4. 50649600	-3. 32682000	0. 38370900
C	-3. 97756800	-4. 97532000	-3. 09722200
C	-4. 68640100	-2. 90227500	-4. 21607500
C	-3. 74531100	-5. 68615600	-1. 95223700
H	-3. 76818000	-5. 64249500	0. 22129100
H	-3. 84296500	-5. 43426800	-4. 07378000
H	-4. 57781900	-3. 40149200	-5. 17691400
H	-3. 41457800	-6. 71970500	-2. 00320000
C	3. 45066700	-0. 16355700	2. 71474000
H	3. 75161900	-1. 20663400	2. 74463900
C	2. 13028200	0. 16408200	2. 88306300

H	1.39769600	-0.61797600	3.03658100
C	4.43191200	0.84222600	2.47927400
H	5.47336100	0.55835200	2.35622700
C	4.05403500	2.15461200	2.39052000
H	4.78813100	2.93160500	2.19196500
C	-5.88748600	1.13487000	-4.11358100
H	-6.17079300	2.18393100	-4.09691300
C	-5.78184700	0.45693200	-5.36103100
H	-6.00078500	0.98691900	-6.28399400
C	-5.39171400	-0.85464300	-5.38990500
H	-5.29117800	-1.38299900	-6.33518300
C	-5.62329700	0.48407200	-2.93561700
H	-5.68785600	1.02621000	-1.99950400
C	-0.02887700	3.64051800	-1.98217400
C	-0.90255200	4.36828500	-2.81581600
C	-0.43452600	3.44961100	-0.65799700
C	-2.10095400	4.89777700	-2.34603000
H	-0.64719000	4.53561700	-3.85875600
C	-1.63910600	3.97444400	-0.17822200
H	0.17972800	2.88621100	0.03533600
C	-2.47357300	4.70784100	-1.01431300
H	-2.74076300	5.45925000	-3.02220800
H	-1.91697500	3.79563000	0.85368600
H	-3.40575800	5.12063900	-0.63821400
C	3.09989600	5.15012100	-2.64362700
C	2.80564800	6.19046300	-1.83333500
C	-1.49126000	-1.03769100	-3.42319300
H	-1.33308900	-1.39356700	-4.45086100
H	-1.00516000	-1.73536500	-2.74007500
H	-2.56073800	-1.07805500	-3.22043400
C	3.84600700	7.05350700	-1.14863900
H	3.56791900	7.21026000	-0.09719800
H	4.85590300	6.64184400	-1.16249500
H	3.88481300	8.05297200	-1.60593700
C	1.29092600	-0.54608100	-3.31925200
H	2.34485300	-0.27708600	-3.34020100
H	1.09938100	-1.21009000	-2.47075800
H	1.06869100	-1.14827400	-4.21372600
C	4.51638000	4.80685000	-3.06797400
H	4.74187300	3.74175200	-2.93912600
H	4.63570600	5.01680800	-4.14166400
H	5.28600800	5.37463800	-2.54368400
C	-2.00706900	1.39314200	-3.90718400
H	-2.95938800	1.34429500	-3.37548400

H	-1.67232500	2.42603600	-3.89164600
H	-2.19678800	1.09312100	-4.94654000
C	1.40420900	6.65936700	-1.51497800
H	1.36564000	7.75698300	-1.54581200
H	0.64682600	6.27749100	-2.19843600
H	1.10070400	6.36591200	-0.50021500

TS-1-2-7RS-2

1 imaginary frequency

H = -5472.458118

G = -5472.671731

E(M06-2X-DCM) = -5473.439095

O	-1.83317400	1.00034400	1.72934700
O	-3.27911500	-0.98007000	0.82539000
P	-1.82159000	-0.26777200	0.70184200
O	-1.60908500	0.36268400	-0.66946500
N	-0.83755300	-1.36711000	1.31386200
S	0.16638700	-2.36837600	0.63042300
C	-0.87989100	-3.76772300	-0.03306400
F	-0.09434500	-4.64909000	-0.65750300
F	-1.52403900	-4.37658400	0.96144600
F	-1.77587700	-3.28689600	-0.90866900
C	1.18698000	3.18644200	-2.59513900
C	0.95737300	2.04692800	-3.67926000
H	0.24846600	2.46393700	-4.40422500
H	1.91416800	1.93417400	-4.19744300
C	0.50214100	0.63006000	-3.35610600
C	2.21622400	2.76269400	-1.49800000
H	2.04516100	3.35605900	-0.59453100
H	3.21144100	3.02211800	-1.85389700
N	2.30955500	1.35266400	-1.13438500
C	3.49204900	0.64683300	-1.18960800
N	3.38547000	-0.59859500	-0.63663200
C	4.37877300	-1.58940000	-0.48375500
C	5.68699800	-1.30049000	-0.08294200
C	3.99155700	-2.92594600	-0.65354800
C	6.58528100	-2.34284200	0.14657200
C	4.90451300	-3.95418300	-0.42989200
H	2.97351300	-3.15773000	-0.94358200
C	6.21037100	-3.67423200	-0.02648500
H	6.91522600	-4.47521600	0.15985400
C	4.49603800	-5.38092800	-0.68430200
C	7.94327800	-2.00192600	0.69683200
F	3.16541400	-5.56018300	-0.55218600

F	5.11113800	-6.23572500	0.16366500
F	4.82422400	-5.77447400	-1.93895100
F	8.81817700	-3.02242300	0.57616900
F	7.87051100	-1.70007200	2.02169700
F	8.48265800	-0.92573000	0.08779100
S	4.88415100	1.22213400	-1.95129300
C	1.90045300	4.35555300	-3.39780900
H	2.68381800	3.87861400	-3.98759000
H	1.18824700	4.76783000	-4.12241200
H	5.99330000	-0.27472000	0.06363200
C	-0.82714300	0.23183800	-3.16797200
H	2.43947100	-0.94883800	-0.46415400
O	1.05059100	-2.98896900	1.61371700
H	1.60506500	0.99012400	-0.50081200
O	0.79595100	-1.80978300	-0.60304200
H	-0.97414700	0.29461200	-1.79013100
C	-7.02639500	0.91096400	0.89167400
C	-6.16160000	1.01502700	1.97412200
C	-4.93955200	0.32191700	1.98991300
C	-5.41310800	-0.53947100	-0.24771100
C	-6.66398500	0.10174400	-0.18078300
C	-1.75346900	0.74212100	3.11141700
C	-2.88887000	0.28931100	3.77673100
C	-2.76440100	-0.20825800	5.08336200
C	-1.55282900	-0.12344100	5.75916000
C	-0.47277000	0.49305900	5.12950500
C	-0.53731100	0.93276600	3.79571100
H	-7.35696900	-0.04221200	-1.00354200
H	0.46085000	0.62781800	5.66696300
C	-4.36423900	0.35962100	3.40406500
C	-4.97159100	1.71168700	3.91407300
H	-4.99908400	1.77017400	5.00596500
H	-4.34491200	2.53550700	3.55266100
H	-3.95587000	-1.78098100	6.00814900
H	-4.54123200	-0.15286400	6.32860200
C	-4.53247200	-0.36312900	0.84296700
H	-7.98417300	1.42502800	0.89155200
H	-1.45043500	-0.50443600	6.77194000
C	-6.36358000	1.78737900	3.25799800
H	-7.13170300	1.31695700	3.88734000
H	-6.69352700	2.81728500	3.07912900
C	-4.07829000	-0.78808000	5.56076800
C	-4.92360900	-0.82025200	4.26824900
H	-5.99922700	-0.73286100	4.44932100

H	-4.74950200	-1.76088200	3.73330300
C	0.64270900	1.66491800	3.23550800
C	0.54413800	3.06399700	3.01720700
C	1.89294400	1.01132300	3.09735900
C	-0.65846400	3.80962200	3.24436800
C	1.71374900	3.80574900	2.59931700
C	3.06541200	1.77806200	2.73503100
C	-0.71512400	5.16300100	3.03279400
H	-1.53650800	3.28839200	3.60885000
C	1.60630600	5.21402400	2.36927900
C	2.93900000	3.14469600	2.47189700
C	0.42705400	5.87797000	2.57427200
H	-1.64096300	5.70009900	3.22113100
H	2.49501200	5.74905800	2.04291600
H	3.82190900	3.71358500	2.18770300
H	0.36119400	6.94898000	2.40441000
C	-5.13626100	-1.41770300	-1.42617900
C	-4.92221200	-2.80886800	-1.24067500
C	-5.22400100	-0.88326300	-2.73996100
C	-4.93626400	-3.43844100	0.04551000
C	-4.72211300	-3.66118500	-2.39120600
C	-5.06756300	-1.75988700	-3.88004900
C	-4.71479700	-4.78279700	0.18811100
H	-5.13599900	-2.83773300	0.92424600
C	-4.47928000	-5.05757100	-2.19901300
C	-4.80045000	-3.11571800	-3.67464800
C	-4.46776900	-5.60655000	-0.94623000
H	-4.72945500	-5.22875000	1.17867000
H	-4.31452700	-5.67557600	-3.07839800
H	-4.66900600	-3.76692500	-4.53644800
H	-4.28499500	-6.66903700	-0.81186100
C	3.29895800	-0.98088700	3.24292500
H	3.38979000	-2.05154400	3.39777000
C	2.06197200	-0.39395000	3.31671500
H	1.19174900	-1.00478000	3.52173100
C	4.45850700	-0.21127600	2.94106500
H	5.43062700	-0.69348500	2.89516300
C	4.33698000	1.12635700	2.67541200
H	5.20823800	1.72386800	2.41819500
C	-5.59643300	0.97405200	-4.29348900
H	-5.78607600	2.03078200	-4.46181500
C	-5.46534300	0.09910800	-5.40832600
H	-5.57143400	0.48887100	-6.41701500
C	-5.19492500	-1.22639400	-5.20118400

H	-5.07939400	-1.90715400	-6.04135700
C	-5.46802500	0.50403200	-3.01169700
H	-5.54344400	1.19669800	-2.18197700
C	-0.16920400	3.66388400	-2.03936600
C	-1.04690600	4.40633000	-2.85518600
C	-0.60203600	3.37381600	-0.74151000
C	-2.28166200	4.85147600	-2.39099600
H	-0.77246700	4.64196200	-3.87897100
C	-1.84628600	3.80711600	-0.27199600
H	0.01889000	2.79885300	-0.06398400
C	-2.68878500	4.55408600	-1.08888900
H	-2.92596100	5.42808700	-3.05000900
H	-2.14335500	3.54673500	0.73711700
H	-3.65270300	4.89613400	-0.72154600
C	2.49914000	5.50432100	-2.59504200
C	3.83080200	5.74329800	-2.55368900
C	-1.17833900	-1.25074000	-3.35605500
H	-1.12512500	-1.51571400	-4.42140300
H	-0.52616900	-1.92394600	-2.80081800
H	-2.20218200	-1.43052600	-3.02246800
C	4.45496800	6.86475200	-1.74631000
H	4.84037700	7.65564300	-2.40623300
H	3.78301500	7.32792300	-1.02266100
H	5.32128700	6.48194300	-1.19057200
C	1.55581200	-0.42824300	-3.51819300
H	2.56829100	-0.02540800	-3.51149700
H	1.46865000	-1.22032300	-2.77255500
H	1.38692700	-0.90793000	-4.49622000
C	1.49201100	6.40168200	-1.89923000
H	0.63063500	6.58652700	-2.55080900
H	1.08722200	5.94911300	-0.98480900
H	1.90829200	7.37436500	-1.63189100
C	-1.98392700	1.14426600	-3.57360300
H	-2.86870300	0.91622400	-2.97917300
H	-1.76824600	2.20206700	-3.45245300
H	-2.24160900	0.95062000	-4.62406800
C	4.89535500	4.95485900	-3.28837800
H	5.47970400	4.34125000	-2.59018000
H	4.51922000	4.28469900	-4.06240400
H	5.60076700	5.64772700	-3.76722500

TS-1-2-7RR

l imaginary frequency

H = -5472.458301

G = -5472.670896

E(M06-2X-DCM) = -5473.446958

O	-1.85913600	0.45311100	1.87264400
O	-3.13921800	-1.30495800	0.40048200
P	-1.85809300	-0.30812700	0.43141700
O	-1.97572400	0.81199500	-0.60531300
N	-0.51570700	-1.18732000	0.35681900
S	-0.23761300	-2.62484700	-0.27061800
C	-0.49928500	-3.83022000	1.13727400
F	-0.24448800	-5.06657200	0.70772200
F	0.31155400	-3.55169100	2.16404000
F	-1.76864800	-3.76777700	1.56220500
C	0.93049200	3.23435600	-1.76290700
C	0.87464200	2.33280800	-3.06237000
H	0.42932800	2.95371100	-3.84914300
H	1.91496400	2.15119100	-3.33828600
C	0.17319900	0.99245800	-3.12413700
C	1.30965600	2.37159900	-0.49419500
H	0.41515600	2.24889800	0.11621300
H	2.05106000	2.90430600	0.10212500
N	1.79556800	1.00634800	-0.70319600
C	3.10737100	0.67677100	-0.93221800
N	3.32925700	-0.67476700	-0.83031600
C	4.52202100	-1.41494300	-0.93273000
C	5.78929500	-0.90596000	-0.62418700
C	4.39980800	-2.76780700	-1.29393400
C	6.90323900	-1.74545600	-0.67413900
C	5.52540000	-3.58571700	-1.34774700
H	3.42162800	-3.17571300	-1.52446100
C	6.79142300	-3.08460800	-1.03919400
H	7.66552100	-3.72194900	-1.08418400
C	5.36500800	-5.04495900	-1.68287400
C	8.22715200	-1.17930000	-0.23591500
F	5.15202700	-5.79065300	-0.57283400
F	6.46833600	-5.54515500	-2.28325700
F	4.31872800	-5.26313900	-2.50849700
F	9.25849800	-2.00351700	-0.51674100
F	8.24366000	-0.96796200	1.10767400
F	8.48664900	0.01123500	-0.81446800
S	4.24771800	1.82571300	-1.38337600
H	5.89942400	0.13082900	-0.34221300
C	-1.21529200	0.80595500	-3.15839700
H	2.51179400	-1.26577300	-0.66736700
O	1.21009000	-2.71465600	-0.55670600

H	1.21231700	0.28639400	-0.27851300
O	-1.17450000	-3.06284600	-1.30995800
H	-1.38508600	0.77656000	-1.80794300
C	-7.02970300	-0.04896000	1.39431000
C	-6.08043800	-0.28284200	2.38111300
C	-4.80551800	-0.76639400	2.04818100
C	-5.40831400	-0.73274100	-0.31645300
C	-6.69611900	-0.31225200	0.07021900
C	-1.58643000	-0.30429500	3.03476600
C	-2.56978800	-1.16150200	3.52908700
C	-2.23627100	-2.09461800	4.52377900
C	-0.98273000	-2.07213000	5.12118600
C	-0.07790700	-1.08634300	4.73785900
C	-0.34083600	-0.18865700	3.68576400
H	-7.44287600	-0.18507400	-0.70689800
H	0.87755000	-1.00630900	5.24623000
C	-4.07827300	-1.18908800	3.31687500
C	-4.76662100	-0.24542900	4.36335600
H	-4.67932500	-0.62424700	5.38570000
H	-4.27491300	0.73369300	4.32836500
H	-3.10098200	-4.07294100	4.80670100
H	-3.83683800	-2.81786100	5.79679600
C	-4.45290200	-0.90640600	0.70578200
H	-8.02414100	0.30863600	1.64853100
H	-0.72007800	-2.78462000	5.89884300
C	-6.22216700	-0.11387000	3.87619000
H	-6.86261400	-0.89798800	4.30347900
H	-6.67642100	0.84547500	4.14915100
C	-3.39996900	-3.01855500	4.80892400
C	-4.38731000	-2.68107400	3.67141400
H	-5.43574000	-2.83701500	3.94298200
H	-4.17034400	-3.30244300	2.79577100
C	0.68059400	0.87935600	3.44199200
C	0.37441100	2.22281500	3.78584500
C	2.01005300	0.51873400	3.10442200
C	-0.91964700	2.64292100	4.23416000
C	1.41980900	3.22235900	3.75487900
C	3.04844500	1.52515500	3.10551400
C	-1.16672700	3.94013900	4.60260700
H	-1.71639000	1.91135200	4.29900400
C	1.11652300	4.56873600	4.13254600
C	2.72180200	2.84887800	3.40930900
C	-0.13871000	4.92296600	4.54741400
H	-2.15826400	4.22260600	4.94638900

H	1. 91770600	5. 30327700	4. 09782000
H	3. 50819500	3. 60084000	3. 41284100
H	-0. 35270400	5. 94616600	4. 84393800
C	-5. 20987900	-1. 02667200	-1. 76987700
C	-4. 96379000	-2. 35508300	-2. 20366300
C	-5. 45904200	-0. 00163400	-2. 72064300
C	-4. 75158600	-3. 44721700	-1. 30290500
C	-4. 96513200	-2. 65297000	-3. 61932800
C	-5. 48951800	-0. 32423400	-4. 12970700
C	-4. 52054600	-4. 71725200	-1. 76089100
H	-4. 77280400	-3. 26363300	-0. 23598900
C	-4. 71504600	-3. 99170500	-4. 05572700
C	-5. 23875400	-1. 63667900	-4. 53855200
C	-4. 49316000	-4. 99737600	-3. 15582400
H	-4. 35306300	-5. 52277700	-1. 05150600
H	-4. 71026800	-4. 19072200	-5. 12472500
H	-5. 26159900	-1. 87498100	-5. 60009500
H	-4. 30142700	-6. 01034600	-3. 49832400
C	3. 70497700	-1. 15438800	2. 55570100
H	3. 96634700	-2. 18303400	2. 32375800
C	2. 39470200	-0. 82518300	2. 78834100
H	1. 63096700	-1. 58991100	2. 73179600
C	4. 72871000	-0. 16447900	2. 59124500
H	5. 75939800	-0. 44607300	2. 39630500
C	4. 40000500	1. 14057000	2. 83797000
H	5. 16428300	1. 91344500	2. 84454000
C	-5. 95854100	2. 32540100	-3. 29576300
H	-6. 12409100	3. 35346200	-2. 98492800
C	-6. 01539000	1. 99345700	-4. 67919100
H	-6. 23845000	2. 76529100	-5. 41066500
C	-5. 77764000	0. 70619600	-5. 07949100
H	-5. 80608900	0. 43859400	-6. 13324500
C	-5. 68532300	1. 36645200	-2. 35415200
H	-5. 62634400	1. 64537300	-1. 30851200
C	1. 94647000	4. 37554100	-2. 00972700
C	2. 41002300	5. 14807200	-0. 93044300
C	2. 37092500	4. 75842700	-3. 29113200
C	3. 26974100	6. 22839200	-1. 11893900
H	2. 09853000	4. 91448700	0. 08130100
C	3. 23226400	5. 84045300	-3. 48679700
H	2. 05152700	4. 20984400	-4. 16989000
C	3. 69009900	6. 58290700	-2. 40145400
H	3. 61351400	6. 79278800	-0. 25575900
H	3. 54644900	6. 09452400	-4. 49591200

H	4.36475400	7.42171000	-2.55015200
C	-0.49091000	3.90340700	-1.56120500
H	-0.73769800	4.36738300	-2.51853000
H	-1.20872300	3.09302300	-1.40555700
C	-0.71209800	4.91699500	-0.44882000
C	-0.70517200	6.25245000	-0.65918800
C	-1.76204700	-0.56763800	-3.55600200
H	-1.30032400	-1.40444400	-3.03102800
H	-2.83117200	-0.60625200	-3.34910000
H	-1.62910900	-0.72461400	-4.63554800
C	-0.92828900	7.26630800	0.44372200
H	-0.12709500	8.01803100	0.42565600
H	-1.86770500	7.81706700	0.28788700
H	-0.94863200	6.83668300	1.44618500
C	1.05650100	-0.20346900	-3.35718600
H	2.11435400	0.03105400	-3.25728600
H	0.81799400	-1.05073100	-2.70874700
H	0.87212100	-0.55779500	-4.38308300
C	-1.02699100	4.31480000	0.90874500
H	-1.52699100	3.34687400	0.79821200
H	-0.12711300	4.13918200	1.51128100
H	-1.68640400	4.94619900	1.50794400
C	-2.17483500	1.92812100	-3.57261600
H	-3.01658700	2.01077000	-2.88122900
H	-1.70132800	2.90427700	-3.65244000
H	-2.59274900	1.67128300	-4.55340700
C	-0.45832600	6.92825500	-1.98918500
H	-0.45294500	6.25309000	-2.84585400
H	-1.22423000	7.69585900	-2.16903800
H	0.51100600	7.44450200	-1.98258400

TS-1-2-7RR-1

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H = -5472.454084

G = -5472.666116

E(M06-2X-DCM) = -5473.441760

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P	-1.84782800	-0.27943000	0.40807600
O	-1.90267100	0.88580500	-0.58578700
N	-0.52076500	-1.17824600	0.33224700
S	-0.24173300	-2.60371800	-0.31905600
C	-0.50980900	-3.83748300	1.06190700
F	-0.22521400	-5.06135800	0.61565000

F	0.27451700	-3.56444700	2.11039900
F	-1.78905800	-3.80493200	1.46085700
C	1.08870000	3.34407300	-1.87224600
C	0.98499500	2.38537700	-3.12903300
H	0.54554900	2.98121800	-3.93830600
H	2.01573200	2.16384500	-3.41102800
C	0.24965000	1.06067500	-3.13153100
C	1.39512100	2.51351600	-0.56317800
H	0.47816500	2.45123000	0.02365400
H	2.13862100	3.03328700	0.04012800
N	1.83285800	1.12217900	-0.71715900
C	3.13512900	0.73705200	-0.92093000
N	3.31019300	-0.61896900	-0.79300200
C	4.48658000	-1.38971600	-0.88335400
C	5.75538000	-0.91783300	-0.52642900
C	4.34532400	-2.72915200	-1.28333600
C	6.85292300	-1.77887900	-0.56941400
C	5.45473600	-3.57019500	-1.32749700
H	3.36587800	-3.10973900	-1.55038200
C	6.72225500	-3.10531800	-0.97269100
H	7.58337400	-3.76041700	-1.01138200
C	5.27145200	-5.01627000	-1.70527500
C	8.17783800	-1.24748400	-0.09253800
F	4.99684900	-5.78316400	-0.62364800
F	6.38443300	-5.53010600	-2.27575500
F	4.25292700	-5.18692000	-2.57559800
F	9.19158800	-2.10826100	-0.32227600
F	8.15374600	-1.01180400	1.24703700
F	8.49568300	-0.07614400	-0.68135100
S	4.32580200	1.83125300	-1.37542300
H	5.88020100	0.10795300	-0.21274200
C	-1.14265500	0.90159500	-3.13591400
H	2.47471200	-1.18873500	-0.64637200
O	1.20728800	-2.68898000	-0.59927400
H	1.22098000	0.43538300	-0.27941900
O	-1.17410300	-3.02352500	-1.36983100
H	-1.31217600	0.86389800	-1.78351400
C	-7.04578900	-0.02214900	1.29632100
C	-6.11463000	-0.32096600	2.28262800
C	-4.83659900	-0.79294800	1.94383200
C	-5.40185500	-0.62155500	-0.42371500
C	-6.69240800	-0.21218700	-0.03493400
C	-1.63994600	-0.39298400	3.01159900
C	-2.62996700	-1.27610400	3.44024500

C	-2.31436500	-2.25904600	4.39196500
C	-1.07407800	-2.26402900	5.01689700
C	-0.16600200	-1.25478000	4.70711900
C	-0.41155100	-0.30496500	3.69846300
H	-7.42535500	-0.03607800	-0.81567400
H	0.77698700	-1.19587200	5.24132000
C	-4.13345100	-1.29053800	3.19924800
C	-4.83675400	-0.40449800	4.28575200
H	-4.76811300	-0.84105300	5.28625900
H	-4.34125000	0.57292700	4.31422900
H	-3.17898800	-4.25152700	4.54169500
H	-3.93636400	-3.05864800	5.59073500
C	-4.46223600	-0.85735200	0.60104000
H	-8.04161800	0.32816900	1.55513800
H	-0.82480500	-3.01612700	5.76093600
C	-6.28269600	-0.23915100	3.78212000
H	-6.93261800	-1.04479400	4.15114900
H	-6.73931700	0.70417300	4.10278000
C	-3.48120700	-3.19973300	4.60086200
C	-4.44974700	-2.79882500	3.46679400
H	-5.50252200	-2.96686000	3.71323200
H	-4.22023800	-3.37251300	2.56243400
C	0.59450200	0.79122000	3.53407800
C	0.25731100	2.10198900	3.96282000
C	1.93080700	0.48319700	3.17694300
C	-1.03632500	2.45165300	4.47050000
C	1.27055100	3.13387900	3.96441800
C	2.94124300	1.51695100	3.22391800
C	-1.31428500	3.71688900	4.91845300
H	-1.80551000	1.68971600	4.51685400
C	0.93193600	4.44872000	4.41477900
C	2.57808400	2.81669000	3.58506600
C	-0.32215000	4.73695500	4.88284000
H	-2.30275400	3.94612600	5.30747100
H	1.70679100	5.21152800	4.39844200
H	3.34190100	3.59103500	3.61556200
H	-0.56055800	5.73512600	5.23981900
C	-5.18838500	-0.84430000	-1.88773500
C	-4.96306700	-2.15423600	-2.38464800
C	-5.40629500	0.23147400	-2.78833100
C	-4.77989000	-3.29313800	-1.53712600
C	-4.95403600	-2.38124000	-3.81339400
C	-5.42379600	-0.01920400	-4.21214000
C	-4.56802900	-4.54325000	-2.05537400

H	-4.80744300	-3.16166800	-0.46267600
C	-4.72557000	-3.70149500	-4.31323000
C	-5.19471900	-1.31449400	-4.68346200
C	-4.53247300	-4.75461400	-3.46217900
H	-4.42203100	-5.38575700	-1.38534800
H	-4.71335600	-3.84756400	-5.39069200
H	-5.20899200	-1.49889000	-5.75584500
H	-4.35681100	-5.75301700	-3.85270800
C	3.67062900	-1.12054100	2.56919500
H	3.96123700	-2.13193600	2.29970100
C	2.35081700	-0.83534600	2.80467800
H	1.60743100	-1.61667000	2.71324300
C	4.66737900	-0.10605500	2.65098800
H	5.70630800	-0.35502400	2.45578800
C	4.30329700	1.17957900	2.94560100
H	5.04757600	1.97066300	2.98897100
C	-5.85430700	2.59362900	-3.25032200
H	-6.00539000	3.60760900	-2.88987800
C	-5.89752800	2.33329900	-4.64954100
H	-6.09546200	3.14547500	-5.34359800
C	-5.67907000	1.06350000	-5.11188000
H	-5.69858100	0.85026600	-6.17817300
C	-5.61287500	1.58303900	-2.35527700
H	-5.56471200	1.80669100	-1.29583100
C	2.18904600	4.39568800	-2.16687900
C	2.77891300	5.12478000	-1.12010100
C	2.57422100	4.73829600	-3.47217600
C	3.72399000	6.11916500	-1.36179300
H	2.49070800	4.93456100	-0.09238200
C	3.51977100	5.73627600	-3.72107000
H	2.15335300	4.22383600	-4.32875300
C	4.10651500	6.43071000	-2.66666200
H	4.16364000	6.65122300	-0.52195800
H	3.79705700	5.96211000	-4.74758600
H	4.84728600	7.20257600	-2.85675000
C	-0.28629300	4.11239200	-1.70764500
H	-0.54746700	4.47000000	-2.71144700
H	-1.04088400	3.37321000	-1.43241200
C	-0.38865600	5.32569400	-0.79239000
C	-0.95531000	5.28901400	0.43278900
C	-1.72266000	-0.46170700	-3.52488800
H	-1.26216900	-1.31037300	-3.01896900
H	-2.78588500	-0.48358700	-3.28832200
H	-1.62177000	-0.61323000	-4.60851700

C	-1.11813100	6.53053700	1.28313900
H	-2.18121900	6.80044900	1.37109300
H	-0.76388200	6.33838200	2.30443700
H	-0.58505300	7.40176900	0.89857400
C	1.10597400	-0.15636600	-3.35693200
H	2.16893400	0.05429500	-3.25625500
H	0.84677400	-0.99597600	-2.70705200
H	0.91717300	-0.50910300	-4.38278600
C	0.02045300	6.65505300	-1.42145100
H	0.45051400	6.51052000	-2.41459500
H	-0.84787900	7.31876400	-1.53194900
H	0.76978100	7.19524700	-0.83418300
C	-2.08742100	2.04075500	-3.53673800
H	-2.90528300	2.15465500	-2.82133900
H	-1.59293900	3.00310500	-3.64542400
H	-2.54274200	1.78270000	-4.50018000
C	-1.52189900	4.05991000	1.10194800
H	-1.65675600	3.20247500	0.44172600
H	-0.88970400	3.74009700	1.93812000
H	-2.50238800	4.29299900	1.53987800