

Supporting Information

Origin of Stereoselectivity and Multidimensional Quantitative Analysis of Ligand Effects in Yttrium-Catalysed Polymerization of 2-Vinylpyridine

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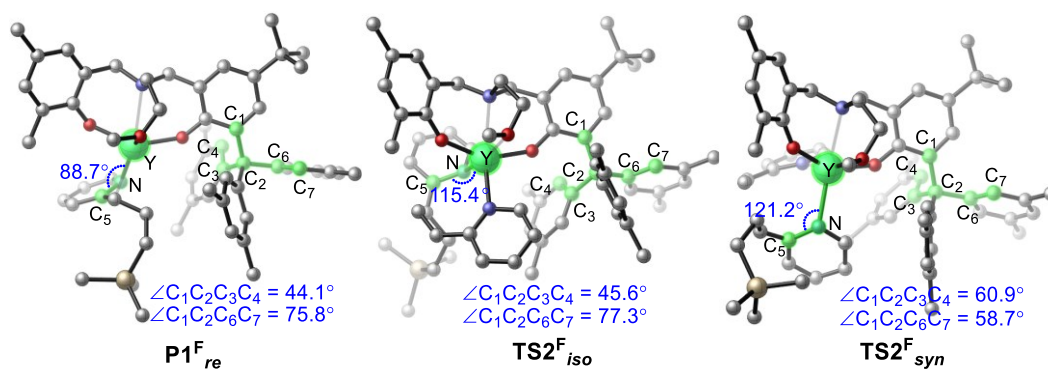


Fig. S1 Geometric parameters for **P1^F_{re}**, **TS2^F_{iso}**, and **TS2^F_{syn}**.

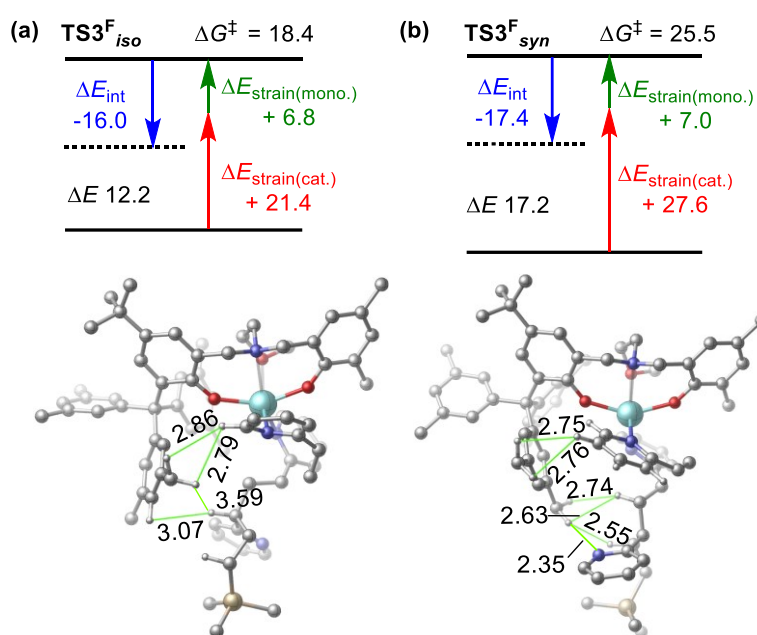


Fig. S2 Activation strain model (kcal mol⁻¹) of **TS3^F_{iso}** and **TS3^F_{syn}**.

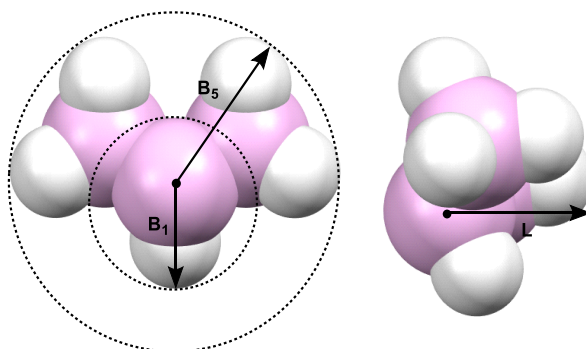


Fig. S3 Parameterization of an isopropyl group using Verloop's Sterimol parameters.

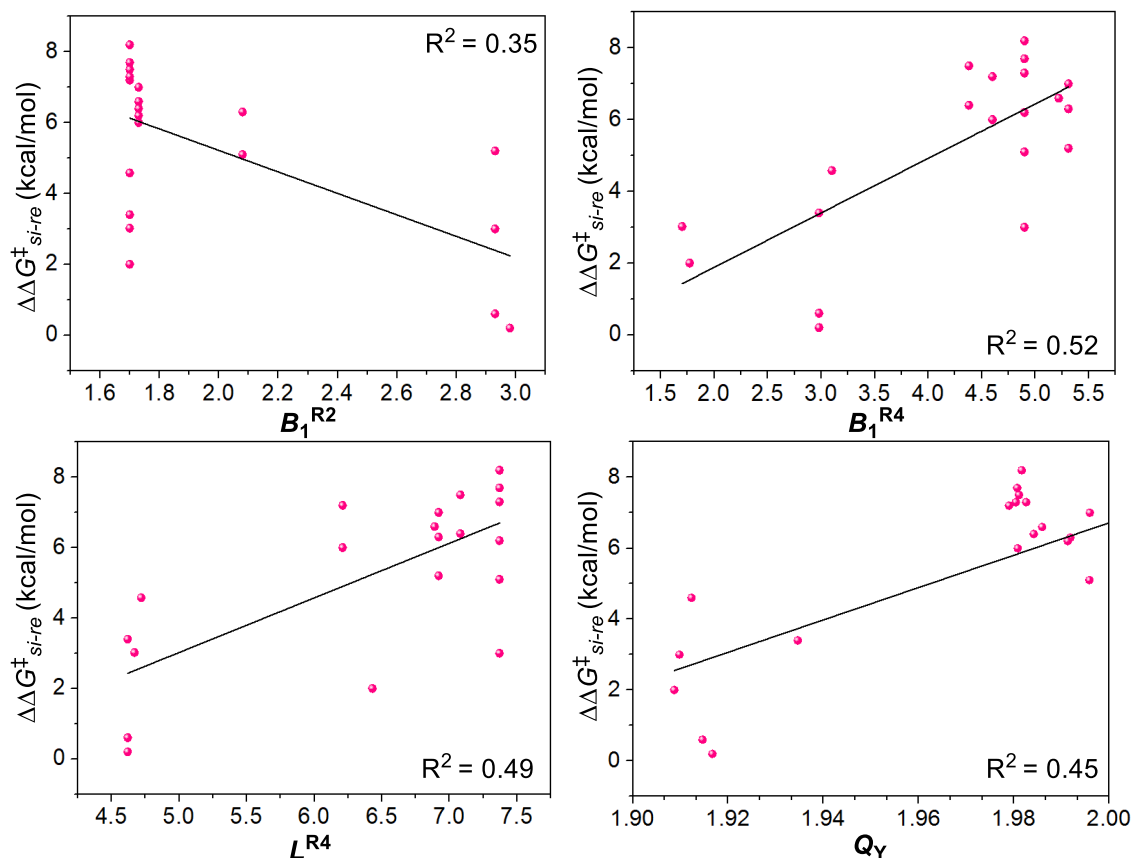


Fig. S4 Representative univariate trends.

Base equation for linear regression:

$$\Delta\Delta G^{\ddagger} = z0 + ax_1 + bx_2 + cx_3 + dx_4 + \dots ex_1x_2 + fx_1x_3 + gx_1x_4 + hx_2x_3 + ix_2x_4 + jx_3x_4 \dots \quad (\text{eq. S1})$$

Equation S1 is the base equation from which all models were derived. A stepwise regression (Syntax: mdl = stepwiselm (_, modelspec)) was performed, stepwiselm uses forward and backward stepwise regression to determine a final model. At each step, the function searches for terms to add the model to or remove from the model, based on the value of the 'Criterion' argument. Multivariate regression was performed using MATLAB.

Table S1. Computed descriptors and energy values (free energies in kcal mol⁻¹) for the second 2VP insertion for the catalysts A–U (see Figs 1 and 8).

	R ²			R ⁴			NPA Charge			%V _{Bur}	ΔG_{DFT}	$\Delta G_{\text{predicted}}$
	$L^{\text{R}2}$	$B_1^{\text{R}2}$	$B_5^{\text{R}2}$	$L^{\text{R}4}$	$B_1^{\text{R}4}$	$B_5^{\text{R}4}$	Q_{Y}	$Q_{\text{O}1}$	$Q_{\text{O}2}$			
A	4.62	2.98	6.07	4.62	2.98	6.07	1.92	-0.92	-0.92	89.7	0.2	0.0
B	4.41	2.93	3.35	4.62	2.98	6.07	1.91	-0.92	-0.92	89.7	0.6	0.2
C	3.09	1.70	2.19	4.62	2.98	6.07	1.93	-0.91	-0.90	88.7	3.4	3.9
D	4.41	2.93	3.35	7.37	4.90	6.99	2.00	-0.93	-0.92	90.7	3.0	4.0
E	4.41	2.93	3.35	6.92	5.31	8.83	2.03	-0.95	-0.93	90.4	5.2	4.8
F	3.09	1.70	2.19	7.37	4.90	6.99	1.98	-0.93	-0.92	89.4	8.2	7.7
G	4.39	2.08	3.34	7.37	4.90	6.99	2.00	-0.93	-0.92	90.0	5.1	6.6
H	4.46	1.73	3.32	6.21	4.60	7.54	1.98	-0.93	-0.91	90.0	6.0	7.0
I	4.39	2.08	3.34	6.92	5.31	8.83	1.99	-0.93	-0.92	89.4	6.3	7.4
J	4.46	1.73	3.32	7.37	4.90	6.99	1.99	-0.93	-0.92	89.9	6.2	7.6
K	4.46	1.73	3.32	7.08	4.38	8.33	1.98	-0.93	-0.92	89.9	6.4	6.6
L	4.46	1.73	3.32	6.89	5.22	8.76	1.99	-0.93	-0.91	89.2	6.6	8.2
M	4.46	1.73	3.32	6.92	5.31	8.83	2.00	-0.91	-0.93	89.1	7.0	8.4
N	3.09	1.70	2.19	6.21	4.60	7.54	1.98	-0.92	-0.91	89.9	7.2	7.1
O	3.09	1.70	2.19	7.08	4.38	8.33	1.98	-0.92	-0.91	90.0	7.5	6.7
P	3.09	1.70	2.19	4.67	1.70	6.03	1.91	-0.91	-0.90	86.6	3.0	1.4
Q	3.09	1.70	2.19	4.72	3.10	3.66	1.91	0.38	-0.91	88.5	4.6	4.1
R	3.09	1.70	2.19	6.43	1.77	3.16	1.91	-0.91	-0.90	86.3	2.0	1.5
S	3.09	1.70	2.19	7.37	4.90	6.99	1.98	-0.93	-0.91	89.4	7.7	7.7
T	3.09	1.70	2.19	7.37	4.90	6.99	1.98	-0.93	-0.91	89.8	7.3	7.7
U	3.09	1.70	2.19	7.37	4.90	6.99	1.98	-0.92	-0.91	89.6	7.3	7.7

Examples of input files:

(1) Optimization and frequency calculations

#p Opt Freq ONIOM(B3PW91/GenECP:HF/LanL2MB)

Optimization complex F

0 1 0 1 0 1

Y 0 1.89459800 -0.42434400 -0.02581700 H
N 0 2.14923800 2.26535300 0.23077600 H
C 0 2.17440000 2.92694000 -1.08246500 H
H 0 3.22004000 3.03409900 -1.38736600 H
H 0 1.74052700 3.93936600 -1.03856600 H
C 0 1.42215100 2.11074400 -2.12325000 H
H 0 0.36584900 2.03315600 -1.86573300 H

H O 1.50478500 2.57364500 -3.11545900 H
 O O 1.91394500 0.76452300 -2.18771400 H
 C O 3.03139200 0.59034200 -3.06051200 H
 H O 3.27288300 -0.47277500 -3.05256200 H
 H O 3.90137600 1.15995100 -2.71780200 H
 H O 2.75399000 0.89602500 -4.07644600 H
 O O -0.10940800 0.23188100 0.50424900 H
 C O -0.90058900 1.27865900 0.35540900 H
 C O -0.36967200 2.58037700 0.54320400 H
 C O 1.02589700 2.73245800 1.08043300 H
 H O 1.19170100 3.79506700 1.33311400 H
 H O 1.10866100 2.16888400 2.02102200 H
 C O -2.27844700 1.15734700 0.01510400 H
 C O -3.03205300 2.32703000 -0.14081400 H
 H O -4.08132800 2.21477800 -0.36609900 H
 C O -2.51106300 3.61790800 -0.00331700 H
 C O -1.16164800 3.70904700 0.35285700 H
 H O -0.70586200 4.68293500 0.51615400 H
 C O -3.36030300 4.91990700 -0.19178100 L H 23 0.0000
 C O -4.82326400 4.60964700 -0.60218800 L
 H O -5.36836800 5.53874400 -0.73728000 L
 H O -5.33168500 4.03050800 0.16146100 L
 H O -4.86068700 4.05843500 -1.53603400 L
 O O 4.03659500 -0.07531000 0.01962400 H
 C O 4.94924300 0.87259000 -0.11916400 H
 C O 4.68730800 2.19638400 0.30085400 H
 C O 3.39787600 2.51384700 1.00196600 H
 H O 3.31102800 1.90584000 1.91405800 H
 H O 3.42075000 3.56831400 1.32923900 H
 C O 6.21516300 0.58468700 -0.69646900 H
 C O 7.14821100 1.60775100 -0.84914400 H
 H O 8.11110200 1.36782600 -1.29495000 H
 C O 6.89470100 2.92745600 -0.44816000 H
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 H O 5.42445600 4.20459200 0.46141100 H
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 H O -1.70990500 6.08836600 -1.04398600 L
 H O -2.69196400 5.25990300 -2.24598500 L
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 C O 1.68758000 -2.52250800 -1.18759200 H
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 H O 1.93780300 -2.27153500 -2.23684200 H
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H O 4.80318500 -3.71294100 -1.68165400 H
 H O 4.68650000 -3.43809700 0.06021500 H
 H O 4.80386000 -5.09370100 -0.57297300 H
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 H O 2.45604900 -5.12125000 -3.21301800 H
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 H O 0.74936800 -5.13054300 0.70445300 H
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 O O 2.20918400 -1.03299300 2.27719900 H
 H O 0.41075700 -0.37739800 3.00669200 H
 H O 1.70856900 -0.55730000 5.47231000 H
 H O 4.21553100 0.11329300 4.19085600 H
 H O 4.24473100 -1.16834800 2.15454200 H
 H O 3.88681100 -1.41988700 4.99905900 H
 H O 3.44055500 -2.53923500 2.97308600 H
 H O 2.00123500 0.81913300 4.40381200 H
 H O 0.95961400 -1.95077400 3.64495400 H
 C O 7.95510100 4.02253100 -0.62909200 L H 40 0.0000
 H O 8.24666400 4.11525800 -1.67296500 L
 H O 7.57568200 4.98333800 -0.29594900 L
 H O 8.85152900 3.79498800 -0.05608600 L
 C O 6.52244200 -0.84935600 -1.13544400 L H 37 0.0000
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 H O 5.80901400 -1.19004200 -1.88258100 L
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 H O -2.38947900 6.00884100 1.44703400 L

H 0 -3.98098300 6.62407900 1.02516700 L
 H 0 -3.82981500 5.12409400 1.93369100 L
 C 0 -2.36786100 -1.14528500 -1.19953700 L
 C 0 -2.79688700 -2.46416500 -1.35233000 L
 C 0 -1.58367500 -0.59564100 -2.21074500 L
 C 0 -2.41255700 -3.23568000 -2.44026000 L
 H 0 -3.46776100 -2.89306900 -0.62213600 L
 C 0 -1.19887900 -1.34366500 -3.32125300 L
 H 0 -1.31158900 0.44795900 -2.16390200 L
 C 0 -1.60528400 -2.66730200 -3.41807300 L
 H 0 -1.31095300 -3.25510000 -4.27742900 L
 C 0 -2.66609100 -0.89082800 1.39463600 L
 C 0 -2.09526700 -2.12965900 1.63586000 L
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 H 0 -2.97696200 -4.97736800 -3.59982800 L
 H 0 -2.14051200 -5.35561100 -2.10116400 L
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 C 0 -1.36645100 -4.01736300 3.15903700 L
 H 0 -1.17708900 -4.19579500 4.21256100 L
 H 0 -2.05817700 -4.77961800 2.80668000 L
 H 0 -0.43543000 -4.14186500 2.61405300 L
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 H 0 -4.15182500 -0.21757100 5.53191900 L
 H 0 -2.52027300 0.41100700 5.68746500 L
 H 0 -3.68829900 1.24287000 4.66461600 L

C H O N 0

6-31g(d)

Si 0

MWB10

d 1 1.0

0.284 1.0

Y 0

MWB28

Si 0

MWB10

Y 0

MWB28

(2) Single-point calculation

#p M06/GenECP SCRF(SMD, Solvent=toluene)

Single point

O 1

Y 1.89459800 -0.42434400 -0.02581700

N 2.14923800 2.26535300 0.23077600

C 2.17440000 2.92694000 -1.08246500

H 3.22004000 3.03409900 -1.38736600

H 1.74052700 3.93936600 -1.03856600

C 1.42215100 2.11074400 -2.12325000

H 0.36584900 2.03315600 -1.86573300

H 1.50478500 2.57364500 -3.11545900

O 1.91394500 0.76452300 -2.18771400

C 3.03139200 0.59034200 -3.06051200

H 3.27288300 -0.47277500 -3.05256200

H 3.90137600 1.15995100 -2.71780200

H 2.75399000 0.89602500 -4.07644600

O -0.10940800 0.23188100 0.50424900

C -0.90058900 1.27865900 0.35540900

C -0.36967200 2.58037700 0.54320400

C 1.02589700 2.73245800 1.08043300

H 1.19170100 3.79506700 1.33311400
 H 1.10866100 2.16888400 2.02102200
 C -2.27844700 1.15734700 0.01510400
 C -3.03205300 2.32703000 -0.14081400
 H -4.08132800 2.21477800 -0.36609900
 C -2.51106300 3.61790800 -0.00331700
 C -1.16164800 3.70904700 0.35285700
 H -0.70586200 4.68293500 0.51615400
 C -3.36030300 4.91990700 -0.19178100
 C -4.82326400 4.60964700 -0.60218800
 H -5.36836800 5.53874400 -0.73728000
 H -5.33168500 4.03050800 0.16146100
 H -4.86068700 4.05843500 -1.53603400
 O 4.03659500 -0.07531000 0.01962400
 C 4.94924300 0.87259000 -0.11916400
 C 4.68730800 2.19638400 0.30085400
 C 3.39787600 2.51384700 1.00196600
 H 3.31102800 1.90584000 1.91405800
 H 3.42075000 3.56831400 1.32923900
 C 6.21516300 0.58468700 -0.69646900
 C 7.14821100 1.60775100 -0.84914400
 H 8.11110200 1.36782600 -1.29495000
 C 6.89470100 2.92745600 -0.44816000
 C 5.65317300 3.19386300 0.12679600
 H 5.42445600 4.20459200 0.46141100
 C -2.72255100 5.79934400 -1.30414400
 H -1.70990500 6.08836600 -1.04398600
 H -2.69196400 5.25990300 -2.24598500
 H -3.30457900 6.70459400 -1.44942800
 C 1.68758000 -2.52250800 -1.18759200
 H 0.59619400 -2.69760900 -1.19946600
 H 1.93780300 -2.27153500 -2.23684200
 Si 2.46973400 -4.19181600 -0.86952600
 C 4.37029100 -4.10201500 -0.75214300
 H 4.80318500 -3.71294100 -1.68165400
 H 4.68650000 -3.43809700 0.06021500
 H 4.80386000 -5.09370100 -0.57297300
 C 2.07644800 -5.46498400 -2.24251000
 H 2.45604900 -5.12125000 -3.21301800
 H 2.52546900 -6.44496200 -2.03663800
 H 0.99339200 -5.60576800 -2.34538600
 C 1.83019500 -4.95355700 0.76008800
 H 0.74936800 -5.13054300 0.70445300
 H 2.31366800 -5.91596100 0.96779200

H 2.01805900 -4.29173300 1.61452600
 C -2.92629800 -0.28243400 -0.02348700
 C -4.46655700 -0.21789000 -0.31551300
 C -5.43302000 -0.66812900 0.56479700
 C -4.89189200 0.25453400 -1.56656600
 C -6.79328200 -0.63559600 0.23794800
 H -5.15041700 -1.06311500 1.52825600
 C -6.22727400 0.30036200 -1.91259100
 H -4.15319600 0.58936700 -2.28095500
 C -7.17985000 -0.14782700 -0.99339300
 H -8.22881300 -0.11795400 -1.25672600
 C 1.27432900 -0.93676700 3.36803900
 C 2.07604800 -0.27015500 4.48289000
 C 3.52901200 -0.73747800 4.22251300
 C 3.46351700 -1.44827900 2.86165400
 O 2.20918400 -1.03299300 2.27719900
 H 0.41075700 -0.37739800 3.00669200
 H 1.70856900 -0.55730000 5.47231000
 H 4.21553100 0.11329300 4.19085600
 H 4.24473100 -1.16834800 2.15454200
 H 3.88681100 -1.41988700 4.99905900
 H 3.44055500 -2.53923500 2.97308600
 H 2.00123500 0.81913300 4.40381200
 H 0.95961400 -1.95077400 3.64495400
 C 7.95510100 4.02253100 -0.62909200
 H 8.24666400 4.11525800 -1.67296500
 H 7.57568200 4.98333800 -0.29594900
 H 8.85152900 3.79498800 -0.05608600
 C 6.52244200 -0.84935600 -1.13544400
 H 6.46048800 -1.53446000 -0.29371000
 H 5.80901400 -1.19004200 -1.88258100
 H 7.51980600 -0.91557400 -1.55873300
 C -3.38937800 5.72066600 1.14061600
 H -2.38947900 6.00884100 1.44703400
 H -3.98098300 6.62407900 1.02516700
 H -3.82981500 5.12409400 1.93369100
 C -2.36786100 -1.14528500 -1.19953700
 C -2.79688700 -2.46416500 -1.35233000
 C -1.58367500 -0.59564100 -2.21074500
 C -2.41255700 -3.23568000 -2.44026000
 H -3.46776100 -2.89306900 -0.62213600
 C -1.19887900 -1.34366500 -3.32125300
 H -1.31158900 0.44795900 -2.16390200
 C -1.60528400 -2.66730200 -3.41807300

H -1.31095300 -3.25510000 -4.27742900
 C -2.66609100 -0.89082800 1.39463600
 C -2.09526700 -2.12965900 1.63586000
 C -3.05119400 -0.12315300 2.50481100
 C -1.94771400 -2.62211400 2.93803200
 H -1.75666500 -2.74511900 0.81723900
 C -2.90335300 -0.58130100 3.79876900
 H -3.48590500 0.85267100 2.34088700
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 H -2.24699400 -2.22335200 5.01530800
 C -7.82309600 -1.14234600 1.24610400
 H -8.82815500 -1.06632000 0.84427200
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 C -6.67101500 0.82841200 -3.27538600
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 H -7.28864400 1.71669500 -3.16197600
 H -5.81376200 1.08565300 -3.88878300
 C -0.36804300 -0.71850200 -4.44036900
 H 0.60555800 -1.19715700 -4.51014600
 H -0.86480000 -0.83789700 -5.40044900
 H -0.21634100 0.34101300 -4.26420800
 C -2.86896300 -4.68844200 -2.55873700
 H -2.97696200 -4.97736800 -3.59982800
 H -2.14051200 -5.35561100 -2.10116400
 H -3.82024200 -4.83788400 -2.05719200
 C -1.36645100 -4.01736300 3.15903700
 H -1.17708900 -4.19579500 4.21256100
 H -2.05817700 -4.77961800 2.80668000
 H -0.43543000 -4.14186500 2.61405300
 C -3.34247900 0.26737200 4.99046100
 H -4.15182500 -0.21757100 5.53191900
 H -2.52027300 0.41100700 5.68746500
 H -3.68829900 1.24287000 4.66461600

C H O N Si 0

6-311G(d,p)

Y 0

MWB28

Y 0

MWB28

Cartesian coordinates and single-point energies ($E_{(\text{SCF Done})}$, a.u.) obtained at the level of M06(SMD,toluene)/6-311G(d,p)-SDD//ONIOM(B3PW91/6-31g(d)-SDD:HF/LanL2MB) for all of the stationary points as well as the imaginary frequency (IF, cm^{-1}) of transition states.

Cat. F, $E_{(\text{SCF Done})} = -2862.190191$ a.u.

Y	1.894598000	-0.424344000	-0.025817000
N	2.149238000	2.265353000	0.230776000
C	2.174400000	2.926940000	-1.082465000
H	3.220040000	3.034099000	-1.387366000
H	1.740527000	3.939366000	-1.038566000
C	1.422151000	2.110744000	-2.123250000
H	0.365849000	2.033156000	-1.865733000
H	1.504785000	2.573645000	-3.115459000
O	1.913945000	0.764523000	-2.187714000
C	3.031392000	0.590342000	-3.060512000
H	3.272883000	-0.472775000	-3.052562000
H	3.901376000	1.159951000	-2.717802000
H	2.753990000	0.896025000	-4.076446000
O	-0.109408000	0.231881000	0.504249000
C	-0.900589000	1.278659000	0.355409000
C	-0.369672000	2.580377000	0.543204000
C	1.025897000	2.732458000	1.080433000
H	1.191701000	3.795067000	1.333114000
H	1.108661000	2.168884000	2.021022000
C	-2.278447000	1.157347000	0.015104000
C	-3.032053000	2.327030000	-0.140814000
H	-4.081328000	2.214778000	-0.366099000
C	-2.511063000	3.617908000	-0.003317000
C	-1.161648000	3.709047000	0.352857000
H	-0.705862000	4.682935000	0.516154000
C	-3.360303000	4.919907000	-0.191781000
C	-4.823264000	4.609647000	-0.602188000
H	-5.368368000	5.538744000	-0.737280000
H	-5.331685000	4.030508000	0.161461000
H	-4.860687000	4.058435000	-1.536034000
O	4.036595000	-0.075310000	0.019624000
C	4.949243000	0.872590000	-0.119164000
C	4.687308000	2.196384000	0.300854000
C	3.397876000	2.513847000	1.001966000
H	3.311028000	1.905840000	1.914058000
H	3.420750000	3.568314000	1.329239000

C	6.215163000	0.584687000	-0.696469000
C	7.148211000	1.607751000	-0.849144000
H	8.111102000	1.367826000	-1.294950000
C	6.894701000	2.927456000	-0.448160000
C	5.653173000	3.193863000	0.126796000
H	5.424456000	4.204592000	0.461411000
C	-2.722551000	5.799344000	-1.304144000
H	-1.709905000	6.088366000	-1.043986000
H	-2.691964000	5.259903000	-2.245985000
H	-3.304579000	6.704594000	-1.449428000
C	1.687580000	-2.522508000	-1.187592000
H	0.596194000	-2.697609000	-1.199466000
H	1.937803000	-2.271535000	-2.236842000
Si	2.469734000	-4.191816000	-0.869526000
C	4.370291000	-4.102015000	-0.752143000
H	4.803185000	-3.712941000	-1.681654000
H	4.686500000	-3.438097000	0.060215000
H	4.803860000	-5.093701000	-0.572973000
C	2.076448000	-5.464984000	-2.242510000
H	2.456049000	-5.121250000	-3.213018000
H	2.525469000	-6.444962000	-2.036638000
H	0.993392000	-5.605768000	-2.345386000
C	1.830195000	-4.953557000	0.760088000
H	0.749368000	-5.130543000	0.704453000
H	2.313668000	-5.915961000	0.967792000
H	2.018059000	-4.291733000	1.614526000
C	-2.926298000	-0.282434000	-0.023487000
C	-4.466557000	-0.217890000	-0.315513000
C	-5.433020000	-0.668129000	0.564797000
C	-4.891892000	0.254534000	-1.566566000
C	-6.793282000	-0.635596000	0.237948000
H	-5.150417000	-1.063115000	1.528256000
C	-6.227274000	0.300362000	-1.912591000
H	-4.153196000	0.589367000	-2.280955000
C	-7.179850000	-0.147827000	-0.993393000
H	-8.228813000	-0.117954000	-1.256726000
C	1.274329000	-0.936767000	3.368039000
C	2.076048000	-0.270155000	4.482890000
C	3.529012000	-0.737478000	4.222513000
C	3.463517000	-1.448279000	2.861654000
O	2.209184000	-1.032993000	2.277199000
H	0.410757000	-0.377398000	3.006692000
H	1.708569000	-0.557300000	5.472310000
H	4.215531000	0.113293000	4.190856000

H	4.244731000	-1.168348000	2.154542000
H	3.886811000	-1.419887000	4.999059000
H	3.440555000	-2.539235000	2.973086000
H	2.001235000	0.819133000	4.403812000
H	0.959614000	-1.950774000	3.644954000
C	7.955101000	4.022531000	-0.629092000
H	8.246664000	4.115258000	-1.672965000
H	7.575682000	4.983338000	-0.295949000
H	8.851529000	3.794988000	-0.056086000
C	6.522442000	-0.849356000	-1.135444000
H	6.460488000	-1.534460000	-0.293710000
H	5.809014000	-1.190042000	-1.882581000
H	7.519806000	-0.915574000	-1.558733000
C	-3.389378000	5.720666000	1.140616000
H	-2.389479000	6.008841000	1.447034000
H	-3.980983000	6.624079000	1.025167000
H	-3.829815000	5.124094000	1.933691000
C	-2.367861000	-1.145285000	-1.199537000
C	-2.796887000	-2.464165000	-1.352330000
C	-1.583675000	-0.595641000	-2.210745000
C	-2.412557000	-3.235680000	-2.440260000
H	-3.467761000	-2.893069000	-0.622136000
C	-1.198879000	-1.343665000	-3.321253000
H	-1.311589000	0.447959000	-2.163902000
C	-1.605284000	-2.667302000	-3.418073000
H	-1.310953000	-3.255100000	-4.277429000
C	-2.666091000	-0.890828000	1.394636000
C	-2.095267000	-2.129659000	1.635860000
C	-3.051194000	-0.123153000	2.504811000
C	-1.947714000	-2.622114000	2.938032000
H	-1.756665000	-2.745119000	0.817239000
C	-2.903353000	-0.581301000	3.798769000
H	-3.485905000	0.852671000	2.340887000
C	-2.355311000	-1.848357000	4.006320000
H	-2.246994000	-2.223352000	5.015308000
C	-7.823096000	-1.142346000	1.246104000
H	-8.828155000	-1.066320000	0.844272000
H	-7.634008000	-2.182713000	1.500223000
H	-7.778430000	-0.564749000	2.166594000
C	-6.671015000	0.828412000	-3.275386000
H	-7.259432000	0.082854000	-3.804811000
H	-7.288644000	1.716695000	-3.161976000
H	-5.813762000	1.085653000	-3.888783000
C	-0.368043000	-0.718502000	-4.440369000

H	0.605558000	-1.197157000	-4.510146000
H	-0.864800000	-0.837897000	-5.400449000
H	-0.216341000	0.341013000	-4.264208000
C	-2.868963000	-4.688442000	-2.558737000
H	-2.976962000	-4.977368000	-3.599828000
H	-2.140512000	-5.355611000	-2.101164000
H	-3.820242000	-4.837884000	-2.057192000
C	-1.366451000	-4.017363000	3.159037000
H	-1.177089000	-4.195795000	4.212561000
H	-2.058177000	-4.779618000	2.806680000
H	-0.435430000	-4.141865000	2.614053000
C	-3.342479000	0.267372000	4.990461000
H	-4.151825000	-0.217571000	5.531919000
H	-2.520273000	0.411007000	5.687465000
H	-3.688299000	1.242870000	4.664616000

2VP, $E_{(\text{SCF Done})} = -325.5171614 \text{ a.u.}$

C	0.482838000	0.248490000	0.000076000
C	-0.457925000	1.289065000	0.000046000
C	-1.813976000	0.980768000	-0.000124000
C	-2.195732000	-0.357166000	-0.000273000
C	-1.188034000	-1.323918000	-0.000255000
N	0.112271000	-1.044962000	-0.000081000
H	-2.559111000	1.772498000	-0.000133000
H	-0.122096000	2.322998000	0.000155000
H	-3.241582000	-0.650109000	-0.000404000
H	-1.446491000	-2.382850000	-0.000358000
C	1.921148000	0.554796000	0.000230000
H	2.178367000	1.613561000	0.000238000
C	2.888831000	-0.367079000	0.000347000
H	2.644320000	-1.425275000	0.000339000
H	3.937800000	-0.085834000	0.000457000

THF, $E_{(\text{SCF Done})} = -232.3542105 \text{ a.u.}$

C	-1.175930000	-0.462655000	0.000000000
O	-0.000007000	-1.251995000	0.000000000
C	1.175922000	-0.462664000	0.000000000
C	0.770963000	1.023651000	0.000000000
C	-0.770953000	1.023657000	0.000000000
H	-1.774682000	-0.718572000	-0.885504000
H	-1.774682000	-0.718571000	0.885505000
H	1.774682000	-0.718595000	0.885498000
H	1.774683000	-0.718596000	-0.885497000
H	1.168052000	1.539584000	0.879522000

H	1.168051000	1.539583000	-0.879524000
H	-1.168033000	1.539598000	0.879522000
H	-1.168033000	1.539598000	-0.879523000

C1^F_{si}, $E_{(\text{SCF Done})} = -2955.37251927$ a.u.

Y	1.869149000	-0.280581000	-0.022778000
N	1.997820000	2.444133000	0.192191000
C	2.017945000	3.077576000	-1.135217000
H	3.062044000	3.189435000	-1.442507000
H	1.574420000	4.086900000	-1.110321000
C	1.276202000	2.232231000	-2.158383000
H	0.223334000	2.136439000	-1.894623000
H	1.344985000	2.684504000	-3.156689000
O	1.796924000	0.899064000	-2.204902000
C	2.892485000	0.728230000	-3.103388000
H	3.159907000	-0.328270000	-3.072524000
H	3.757627000	1.328218000	-2.802059000
H	2.579999000	0.999000000	-4.119294000
O	-0.160136000	0.356794000	0.384922000
C	-1.008096000	1.365589000	0.299808000
C	-0.541120000	2.685074000	0.510612000
C	0.859673000	2.917877000	1.014358000
H	0.984954000	4.000293000	1.197576000
H	0.977296000	2.432572000	1.993361000
C	-2.394022000	1.174121000	0.011879000
C	-3.212099000	2.302802000	-0.057800000
H	-4.267256000	2.150440000	-0.236455000
C	-2.756281000	3.620640000	0.102277000
C	-1.402576000	3.777966000	0.393072000
H	-0.984470000	4.764956000	0.564374000
C	-2.961225000	-0.298181000	-0.075585000
C	-3.764977000	4.811488000	-0.020306000
C	-3.067390000	6.183149000	0.173309000
H	-3.795872000	6.981246000	0.068979000
H	-2.291589000	6.337497000	-0.569511000
H	-2.622555000	6.262358000	1.159771000
C	-4.871602000	4.673071000	1.062767000
H	-5.572679000	5.499514000	0.992714000
H	-4.434792000	4.680194000	2.056780000
H	-5.426018000	3.748747000	0.941005000
O	3.980323000	0.217118000	-0.100500000
C	4.850206000	1.209933000	-0.215292000
C	4.534078000	2.500927000	0.262081000
C	3.232947000	2.736017000	0.972905000

H	3.179292000	2.104785000	1.872558000
H	3.205950000	3.782786000	1.322980000
C	6.116237000	1.005401000	-0.825821000
C	7.001254000	2.075329000	-0.942601000
H	7.965329000	1.899694000	-1.414814000
C	6.697048000	3.361761000	-0.476329000
C	5.452362000	3.546948000	0.123008000
H	5.182008000	4.531405000	0.501521000
C	-4.421128000	4.796890000	-1.429611000
H	-3.665372000	4.894206000	-2.203123000
H	-4.965074000	3.873956000	-1.599282000
H	-5.118412000	5.623494000	-1.529082000
C	1.546547000	-2.273818000	-1.325847000
H	0.526022000	-2.551528000	-0.998393000
H	1.384600000	-1.832680000	-2.327468000
Si	2.418111000	-3.899808000	-1.645411000
C	1.622535000	-4.869429000	-3.090880000
H	0.566932000	-5.082813000	-2.883921000
H	1.663478000	-4.288610000	-4.021099000
H	2.130248000	-5.825607000	-3.271594000
C	2.343566000	-5.053038000	-0.128422000
H	1.302915000	-5.295842000	0.119919000
H	2.866651000	-5.997392000	-0.323467000
H	2.800007000	-4.585735000	0.750733000
C	4.249101000	-3.668044000	-2.130016000
H	4.339490000	-3.053372000	-3.034871000
H	4.814033000	-3.171776000	-1.334049000
H	4.728619000	-4.632397000	-2.338823000
N	2.027041000	-0.942535000	2.552422000
C	2.800155000	-1.768096000	3.302778000
C	1.090795000	-0.215339000	3.190201000
C	2.619603000	-1.863276000	4.691516000
C	3.848241000	-2.610065000	2.710139000
C	0.891568000	-0.226130000	4.565958000
H	0.441425000	0.371438000	2.547826000
C	1.677142000	-1.076348000	5.336106000
H	3.245486000	-2.549806000	5.253637000
H	4.065441000	-3.508954000	3.286733000
C	4.573482000	-2.352073000	1.617429000
H	0.118646000	0.397030000	5.003355000
H	1.551543000	-1.135329000	6.413858000
H	4.460312000	-1.448909000	1.021355000
H	5.336429000	-3.058118000	1.300973000
C	-2.588704000	-0.968073000	1.287369000

C	-1.859924000	-2.142213000	1.413694000
C	-3.007881000	-0.331830000	2.462132000
C	-1.579526000	-2.694111000	2.666200000
H	-1.496141000	-2.654511000	0.537036000
C	-2.749748000	-0.862314000	3.713582000
H	-3.558553000	0.595686000	2.389223000
C	-2.036870000	-2.056169000	3.805536000
H	-1.832010000	-2.482056000	4.778616000
C	-2.416346000	-1.067537000	-1.320171000
C	-2.782737000	-2.398098000	-1.515988000
C	-1.708568000	-0.429851000	-2.335849000
C	-2.416349000	-3.096167000	-2.659538000
H	-3.387196000	-2.897958000	-0.772498000
C	-1.340905000	-1.103321000	-3.496866000
H	-1.478014000	0.620609000	-2.244610000
C	-1.688625000	-2.440299000	-3.643253000
H	-1.407165000	-2.969456000	-4.543965000
C	-4.514770000	-0.310909000	-0.295331000
C	-5.410486000	-0.885620000	0.587284000
C	-5.024816000	0.214732000	-1.492569000
C	-6.783349000	-0.921349000	0.318291000
H	-5.060858000	-1.328839000	1.506644000
C	-6.374385000	0.195004000	-1.780916000
H	-4.341239000	0.643260000	-2.211724000
C	-7.254870000	-0.376554000	-0.858190000
H	-8.314292000	-0.398652000	-1.076567000
C	-3.263663000	-0.166221000	4.972750000
H	-4.258883000	-0.524469000	5.230088000
H	-2.612839000	-0.362391000	5.819572000
H	-3.325698000	0.907780000	4.825136000
C	-0.797378000	-4.003262000	2.758428000
H	0.089047000	-3.969105000	2.130724000
H	-0.490218000	-4.200213000	3.780425000
H	-1.407901000	-4.838947000	2.422277000
C	-2.819575000	-4.560225000	-2.824577000
H	-3.866888000	-4.703454000	-2.572129000
H	-2.662475000	-4.892418000	-3.845629000
H	-2.230234000	-5.196790000	-2.167591000
C	-0.589399000	-0.385806000	-4.616659000
H	0.396393000	-0.821649000	-4.759578000
H	-1.127733000	-0.471358000	-5.557747000
H	-0.467631000	0.667630000	-4.388341000
C	-7.732715000	-1.563750000	1.328114000
H	-8.755370000	-1.542212000	0.966032000

H	-7.456447000	-2.599307000	1.512158000
H	-7.696381000	-1.038598000	2.279925000
C	-6.910605000	0.781003000	-3.085548000
H	-7.458181000	0.029374000	-3.649204000
H	-7.591764000	1.605475000	-2.886722000
H	-6.100598000	1.150115000	-3.705995000
C	7.707614000	4.508882000	-0.614569000
H	7.273388000	5.445774000	-0.280208000
H	8.597963000	4.317087000	-0.019147000
H	8.022682000	4.628860000	-1.648583000
C	6.487106000	-0.388634000	-1.340215000
H	6.583301000	-1.094712000	-0.519082000
H	5.722880000	-0.772539000	-2.011252000
H	7.431325000	-0.359946000	-1.874789000

TS1^F_{si}, $E_{(\text{SCF Done})} = -2955.326476$ a.u., IF = $i249.1$ cm⁻¹

Y	-2.007961000	0.334261000	0.350561000
N	-2.199056000	-2.254394000	-0.039981000
C	-2.153742000	-2.659314000	-1.456870000
H	-3.186352000	-2.738137000	-1.810717000
H	-1.689518000	-3.651404000	-1.573845000
C	-1.401488000	-1.652421000	-2.310112000
H	-0.355225000	-1.598796000	-2.016828000
H	-1.447916000	-1.941475000	-3.369153000
O	-1.933298000	-0.332836000	-2.153044000
C	-3.049297000	-0.079066000	-3.005324000
H	-3.313536000	0.971058000	-2.881827000
H	-3.911747000	-0.700111000	-2.741816000
H	-2.761994000	-0.257649000	-4.049271000
O	0.083767000	-0.293591000	0.437876000
C	0.860960000	-1.320557000	0.151440000
C	0.313896000	-2.627931000	0.201448000
C	-1.072230000	-2.829801000	0.746456000
H	-1.245189000	-3.913651000	0.862166000
H	-1.144289000	-2.389997000	1.752444000
C	2.237971000	-1.185792000	-0.216797000
C	2.934071000	-2.343274000	-0.574486000
H	3.976803000	-2.240032000	-0.837954000
C	2.384985000	-3.634005000	-0.592402000
C	1.061273000	-3.745019000	-0.174168000
H	0.577418000	-4.714963000	-0.114617000
C	2.980168000	0.205330000	-0.062690000
C	3.267734000	-4.849696000	-1.031039000
C	2.472188000	-6.180840000	-1.003274000

H	3.111691000	-6.995565000	-1.328522000
H	1.615655000	-6.140213000	-1.668292000
H	2.122152000	-6.408919000	-0.001936000
C	4.482129000	-4.989601000	-0.070651000
H	5.096728000	-5.836431000	-0.361512000
H	4.144856000	-5.147590000	0.949236000
H	5.101990000	-4.099655000	-0.090379000
O	-4.119862000	0.002422000	0.010755000
C	-5.016472000	-0.922334000	-0.263143000
C	-4.745440000	-2.295773000	-0.055564000
C	-3.459083000	-2.735561000	0.591317000
H	-3.417677000	-2.398943000	1.634335000
H	-3.442171000	-3.839041000	0.625726000
C	-6.288269000	-0.554306000	-0.781602000
C	-7.220199000	-1.541118000	-1.088709000
H	-8.188189000	-1.237827000	-1.482194000
C	-6.956489000	-2.906942000	-0.905276000
C	-5.710111000	-3.254845000	-0.387158000
H	-5.476383000	-4.305865000	-0.222854000
C	3.782698000	-4.623830000	-2.480455000
H	2.949886000	-4.525829000	-3.170241000
H	4.386838000	-3.725408000	-2.546404000
H	4.391464000	-5.464726000	-2.799303000
C	-2.181134000	2.623701000	-0.695661000
H	-1.299930000	2.284077000	-1.266183000
H	-3.085681000	2.113080000	-1.070180000
Si	-2.436177000	4.444033000	-1.106500000
C	-2.876358000	4.648488000	-2.949085000
H	-2.073543000	4.274614000	-3.595120000
H	-3.792914000	4.100760000	-3.199636000
H	-3.041660000	5.704060000	-3.198699000
C	-0.849460000	5.445106000	-0.786171000
H	-0.004387000	5.004847000	-1.328595000
H	-0.971333000	6.477216000	-1.135816000
H	-0.577383000	5.488415000	0.274653000
C	-3.875782000	5.171540000	-0.098142000
H	-4.788927000	4.582158000	-0.244973000
H	-3.663658000	5.196868000	0.976277000
H	-4.087441000	6.198583000	-0.418561000
N	-2.709046000	0.251213000	2.696360000
C	-1.625843000	0.925856000	3.166757000
C	-3.366388000	-0.601474000	3.503390000
C	-1.058342000	0.568171000	4.415711000
C	-1.132589000	1.992602000	2.343991000

C	-2.925919000	-0.917914000	4.773901000
H	-4.267788000	-1.042797000	3.084897000
C	-1.715340000	-0.346174000	5.211405000
H	-0.144266000	1.052482000	4.744178000
H	-0.086450000	2.253343000	2.443910000
C	-1.953880000	2.816065000	1.559074000
H	-3.484856000	-1.607952000	5.397197000
H	-1.311971000	-0.606560000	6.186844000
H	-3.032517000	2.775035000	1.700376000
H	-1.564182000	3.798811000	1.334182000
C	2.780901000	0.655578000	1.424545000
C	2.515056000	1.964598000	1.817223000
C	2.951641000	-0.297094000	2.430584000
C	2.459565000	2.325320000	3.160112000
H	2.345786000	2.730114000	1.077843000
C	2.888196000	0.034516000	3.777755000
H	3.156829000	-1.322562000	2.157849000
C	2.653043000	1.355376000	4.134261000
H	2.616223000	1.631195000	5.179768000
C	2.496104000	1.268097000	-1.101307000
C	3.135535000	2.512551000	-1.154125000
C	1.559315000	0.983411000	-2.084117000
C	2.815266000	3.459113000	-2.111531000
H	3.925016000	2.733019000	-0.450531000
C	1.229229000	1.914342000	-3.071593000
H	1.110642000	0.004012000	-2.124621000
C	1.848717000	3.151785000	-3.066747000
H	1.603509000	3.877566000	-3.830780000
C	4.515271000	0.048184000	-0.360015000
C	5.498001000	0.136243000	0.608051000
C	4.923302000	-0.158264000	-1.687320000
C	6.855221000	0.016218000	0.287372000
H	5.232492000	0.307041000	1.639642000
C	6.254210000	-0.282799000	-2.029918000
H	4.173915000	-0.222187000	-2.463620000
C	7.222364000	-0.193982000	-1.025513000
H	8.268550000	-0.287373000	-1.285024000
C	3.101037000	-1.042186000	4.840611000
H	2.890093000	-0.654978000	5.832192000
H	2.453706000	-1.896572000	4.660064000
H	4.128920000	-1.398663000	4.828001000
C	2.216494000	3.780027000	3.560862000
H	1.799070000	4.345679000	2.734057000
H	1.532137000	3.843278000	4.402304000

H	3.149444000	4.256189000	3.856885000
C	3.512601000	4.818006000	-2.130519000
H	4.432081000	4.789191000	-1.554642000
H	3.751085000	5.116799000	-3.147430000
H	2.870240000	5.584961000	-1.701642000
C	0.210296000	1.567035000	-4.155228000
H	-0.784650000	1.901658000	-3.870672000
H	0.467086000	2.048367000	-5.094381000
H	0.169835000	0.494557000	-4.317358000
C	7.903035000	0.121269000	1.394047000
H	8.905254000	0.030904000	0.988108000
H	7.826654000	1.076642000	1.907905000
H	7.762161000	-0.663321000	2.134014000
C	6.677355000	-0.511783000	-3.479573000
H	7.337167000	0.283530000	-3.818407000
H	7.214963000	-1.451915000	-3.580620000
H	5.813271000	-0.540658000	-4.135187000
C	-8.009858000	-3.966006000	-1.259659000
H	-7.637289000	-4.963606000	-1.049614000
H	-8.921684000	-3.816865000	-0.685335000
H	-8.274111000	-3.917753000	-2.313969000
C	-6.591783000	0.934661000	-0.975507000
H	-6.415507000	1.485445000	-0.054477000
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C	-1.699476000	-2.952113000	-1.779424000
H	-2.747346000	-3.141016000	-2.033426000
H	-1.101412000	-3.759362000	-2.231665000
C	-1.263337000	-1.623379000	-2.378246000
H	-0.211772000	-1.429618000	-2.168781000
H	-1.408334000	-1.621689000	-3.466723000
O	-1.985883000	-0.520306000	-1.807401000
C	-3.268127000	-0.288225000	-2.395374000
H	-3.675914000	0.601674000	-1.914299000
H	-3.947381000	-1.130722000	-2.228920000
H	-3.150820000	-0.103082000	-3.470099000
O	0.366401000	-0.810882000	0.503114000
C	1.308829000	-1.581085000	-0.003750000
C	0.999229000	-2.920959000	-0.330967000
C	-0.291030000	-3.521507000	0.157597000

H	-0.282132000	-4.599858000	-0.078375000
H	-0.316837000	-3.444863000	1.255578000
C	2.637510000	-1.112696000	-0.224027000
C	3.545532000	-1.983763000	-0.826591000
H	4.555440000	-1.631349000	-0.983464000
C	3.236057000	-3.294666000	-1.225224000
C	1.946592000	-3.743541000	-0.944274000
H	1.653237000	-4.763606000	-1.171782000
C	3.030310000	0.334565000	0.276263000
C	4.333225000	-4.175165000	-1.912035000
C	3.794242000	-5.578717000	-2.292880000
H	4.577628000	-6.150448000	-2.780660000
H	2.956046000	-5.504867000	-2.978089000
H	3.475431000	-6.129398000	-1.414064000
C	5.535291000	-4.362683000	-0.944328000
H	6.299209000	-4.979590000	-1.408310000
H	5.214343000	-4.848992000	-0.028161000
H	5.982391000	-3.409048000	-0.684996000
O	-3.724302000	-1.240391000	0.868291000
C	-4.543278000	-2.133432000	0.341603000
C	-4.067170000	-3.411073000	-0.022603000
C	-2.652911000	-3.783050000	0.313710000
H	-2.501495000	-3.700715000	1.399788000
H	-2.485235000	-4.841763000	0.051343000
C	-5.912093000	-1.826322000	0.127527000
C	-6.738924000	-2.781013000	-0.460158000
H	-7.785992000	-2.532707000	-0.620114000
C	-6.275176000	-4.048450000	-0.844587000
C	-4.931614000	-4.340529000	-0.610347000
H	-4.541761000	-5.321828000	-0.877004000
C	4.823516000	-3.476335000	-3.211386000
H	3.998856000	-3.336071000	-3.903670000
H	5.255607000	-2.505217000	-2.995337000
H	5.580326000	-4.081462000	-3.701689000
C	-2.229920000	3.484722000	-1.245224000
H	-1.181863000	3.783895000	-1.093506000
H	-2.185903000	2.586407000	-1.877295000
Si	-3.100200000	4.869764000	-2.225227000
C	-2.195874000	5.130283000	-3.876082000
H	-1.150129000	5.415338000	-3.713206000
H	-2.203422000	4.216183000	-4.481419000
H	-2.670160000	5.924281000	-4.464932000
C	-3.074838000	6.494421000	-1.239798000
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H	-3.550798000	7.303965000	-1.805805000
H	-3.610321000	6.393040000	-0.288909000
C	-4.905344000	4.387827000	-2.581855000
H	-4.962417000	3.457028000	-3.159167000
H	-5.472714000	4.243012000	-1.655284000
H	-5.411445000	5.168687000	-3.161713000
N	-1.972563000	0.614718000	2.761851000
C	-2.612098000	1.683342000	2.175125000
C	-2.323711000	0.207174000	3.991885000
C	-3.714204000	2.272753000	2.852731000
C	-2.151514000	2.025011000	0.854061000
C	-3.337868000	0.793934000	4.725103000
H	-1.759062000	-0.635345000	4.387704000
C	-4.055808000	1.837418000	4.115855000
H	-4.255734000	3.088215000	2.385160000
H	-1.056422000	2.130194000	0.823851000
C	-2.864889000	3.138266000	0.108353000
H	-3.578114000	0.441318000	5.722341000
H	-4.876917000	2.313200000	4.647844000
H	-3.919290000	2.861392000	-0.047480000
H	-2.895817000	4.060551000	0.716773000
C	2.473314000	0.478044000	1.732200000
C	1.795268000	1.595616000	2.195214000
C	2.681560000	-0.577209000	2.631076000
C	1.336883000	1.677761000	3.513110000
H	1.602239000	2.427977000	1.537821000
C	2.235650000	-0.520963000	3.939008000
H	3.205330000	-1.460520000	2.293863000
C	1.562493000	0.620140000	4.375373000
H	1.213859000	0.675820000	5.398118000
C	2.470901000	1.431243000	-0.685655000
C	2.840558000	2.769948000	-0.490921000
C	1.700505000	1.129368000	-1.795039000
C	2.428533000	3.770048000	-1.350040000
H	3.482539000	3.024953000	0.340349000
C	1.277483000	2.121590000	-2.686011000
H	1.452954000	0.101818000	-2.011325000
C	1.637768000	3.433613000	-2.451314000
H	1.322173000	4.209184000	-3.136215000
C	4.587911000	0.521205000	0.269872000
C	5.358160000	0.550084000	1.418281000
C	5.243048000	0.693099000	-0.958818000
C	6.744067000	0.732789000	1.366749000
H	4.895216000	0.438671000	2.386322000

C	6.609908000	0.872715000	-1.037850000
H	4.662682000	0.689349000	-1.870545000
C	7.358979000	0.889477000	0.141148000
H	8.430174000	1.032563000	0.089413000
C	2.481416000	-1.680175000	4.903274000
H	3.136816000	-1.374165000	5.715976000
H	1.547615000	-2.020750000	5.343811000
H	2.943498000	-2.518129000	4.391723000
C	0.625531000	2.942419000	3.992167000
H	-0.036318000	3.328959000	3.222802000
H	0.039784000	2.743210000	4.883777000
H	1.348203000	3.720786000	4.231448000
C	2.828443000	5.224847000	-1.112269000
H	3.581858000	5.297083000	-0.334697000
H	3.226887000	5.669928000	-2.020316000
H	1.966771000	5.814412000	-0.805475000
C	0.446751000	1.737536000	-3.908909000
H	-0.525818000	1.355432000	-3.608475000
H	0.289485000	2.595111000	-4.554676000
H	0.945332000	0.961455000	-4.484818000
C	7.550054000	0.757852000	2.664225000
H	8.602328000	0.930101000	2.463090000
H	7.194091000	1.545702000	3.323920000
H	7.453854000	-0.186023000	3.196024000
C	7.304271000	1.053562000	-2.386276000
H	7.844323000	1.996908000	-2.418186000
H	8.023171000	0.255949000	-2.560001000
H	6.583461000	1.045484000	-3.197264000
C	-7.225422000	-5.071686000	-1.482222000
H	-6.693375000	-5.982477000	-1.737995000
H	-8.032534000	-5.330488000	-0.800205000
H	-7.675542000	-4.674213000	-2.389273000
C	-6.434539000	-0.450695000	0.550393000
H	-6.198361000	-0.253899000	1.593347000
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C	2.040204000	2.820968000	-1.508383000
H	3.079804000	2.880786000	-1.845004000
H	1.610497000	3.833120000	-1.591560000
C	1.267530000	1.874529000	-2.414020000

H	0.217605000	1.831907000	-2.125965000
H	1.328462000	2.203840000	-3.459964000
O	1.762551000	0.534838000	-2.308574000
C	2.851280000	0.242368000	-3.184303000
H	3.100467000	-0.808765000	-3.034550000
H	3.729099000	0.856048000	-2.955450000
H	2.538932000	0.401482000	-4.223710000
O	-0.171920000	0.329011000	0.344892000
C	-0.992608000	1.343446000	0.144529000
C	-0.488075000	2.664937000	0.198896000
C	0.920656000	2.909012000	0.673102000
H	1.070430000	3.999565000	0.766014000
H	1.034842000	2.496543000	1.685701000
C	-2.385144000	1.158473000	-0.113950000
C	-3.170139000	2.293398000	-0.323702000
H	-4.229802000	2.151346000	-0.483570000
C	-2.675455000	3.607207000	-0.325447000
C	-1.317825000	3.760150000	-0.050097000
H	-0.871746000	4.748308000	0.004290000
C	-2.994394000	-0.296302000	-0.011027000
C	-3.648972000	4.802559000	-0.597788000
C	-2.911279000	6.166702000	-0.574493000
H	-3.615827000	6.966506000	-0.780568000
H	-2.131155000	6.204106000	-1.327815000
H	-2.464385000	6.355675000	0.395981000
C	-4.758624000	4.832673000	0.490600000
H	-5.435243000	5.664011000	0.315938000
H	-4.321283000	4.950899000	1.477344000
H	-5.339964000	3.916935000	0.483257000
O	3.974985000	0.068689000	-0.176579000
C	4.865934000	1.016033000	-0.405525000
C	4.582570000	2.364612000	-0.091597000
C	3.294990000	2.716149000	0.597161000
H	3.245016000	2.213564000	1.574359000
H	3.287774000	3.800898000	0.802942000
C	6.128541000	0.705563000	-0.978481000
C	7.038432000	1.729891000	-1.229146000
H	7.999522000	1.472756000	-1.669333000
C	6.763489000	3.073015000	-0.933600000
C	5.524794000	3.362452000	-0.363404000
H	5.279728000	4.393235000	-0.111862000
C	-4.306278000	4.632038000	-1.996322000
H	-3.548520000	4.610165000	-2.773678000
H	-4.877252000	3.711492000	-2.051565000

H	-4.979025000	5.459878000	-2.199987000
C	1.477703000	-2.531279000	-0.934297000
H	0.473079000	-2.745697000	-0.522403000
H	1.263715000	-2.181014000	-1.963290000
Si	2.288186000	-4.203054000	-1.166105000
C	4.110575000	-4.061834000	-1.714128000
H	4.186925000	-3.533388000	-2.673132000
H	4.710609000	-3.506574000	-0.985507000
H	4.564670000	-5.051379000	-1.848167000
C	1.422561000	-5.248967000	-2.513481000
H	1.446071000	-4.734409000	-3.482430000
H	1.901906000	-6.227684000	-2.643593000
H	0.369871000	-5.420306000	-2.258785000
C	2.218971000	-5.256381000	0.426464000
H	2.745156000	-4.794429000	1.269474000
H	1.177770000	-5.415855000	0.733143000
H	2.667211000	-6.243070000	0.256700000
N	2.028254000	-0.468269000	2.631186000
C	3.108756000	-0.725388000	3.411122000
C	0.969340000	0.138983000	3.197664000
C	3.156959000	-0.295079000	4.745045000
C	4.242213000	-1.487489000	2.883395000
C	0.939116000	0.563617000	4.522093000
H	0.121297000	0.297504000	2.538108000
C	2.068466000	0.356499000	5.307813000
H	4.048057000	-0.497758000	5.331523000
H	5.174961000	-1.364998000	3.431387000
C	4.194344000	-2.332072000	1.849684000
H	0.052043000	1.052720000	4.910375000
H	2.098181000	0.685811000	6.343028000
H	3.284173000	-2.534954000	1.290063000
H	5.080383000	-2.868589000	1.526422000
C	-2.627085000	-0.798481000	1.423803000
C	-1.927229000	-1.966468000	1.692030000
C	-3.014753000	-0.007371000	2.511841000
C	-1.641692000	-2.360697000	3.001351000
H	-1.587634000	-2.594882000	0.884025000
C	-2.752985000	-0.381047000	3.818407000
H	-3.542553000	0.917899000	2.326985000
C	-2.066867000	-1.570475000	4.054870000
H	-1.856913000	-1.872837000	5.072088000
C	-2.481921000	-1.235048000	-1.148457000
C	-2.893418000	-2.566769000	-1.171852000
C	-1.755957000	-0.757628000	-2.236219000

C	-2.554921000	-3.417862000	-2.215744000
H	-3.511040000	-2.946232000	-0.370204000
C	-1.414236000	-1.587063000	-3.300295000
H	-1.488641000	0.287113000	-2.279980000
C	-1.808198000	-2.918811000	-3.274608000
H	-1.547834000	-3.568468000	-4.099621000
C	-4.549420000	-0.290683000	-0.218534000
C	-5.453633000	-0.717230000	0.736465000
C	-5.054546000	0.089783000	-1.471480000
C	-6.829377000	-0.745450000	0.481682000
H	-5.108858000	-1.047289000	1.703986000
C	-6.406695000	0.073920000	-1.747738000
H	-4.365013000	0.399518000	-2.243979000
C	-7.295256000	-0.344868000	-0.753530000
H	-8.356826000	-0.362830000	-0.961607000
C	-3.233920000	0.484054000	4.982307000
H	-4.254993000	0.224794000	5.256422000
H	-2.609421000	0.340112000	5.858778000
H	-3.220162000	1.536850000	4.715941000
C	-0.884785000	-3.664175000	3.250869000
H	0.009733000	-3.715202000	2.635477000
H	-0.592686000	-3.749484000	4.292485000
H	-1.506027000	-4.522107000	3.001997000
C	-3.006661000	-4.876858000	-2.191646000
H	-2.420953000	-5.447871000	-1.473874000
H	-4.051260000	-4.953429000	-1.902029000
H	-2.884586000	-5.336294000	-3.167182000
C	-0.638433000	-1.046021000	-4.499827000
H	0.341132000	-1.513256000	-4.567039000
H	-1.167811000	-1.254197000	-5.426649000
H	-0.500116000	0.026901000	-4.419464000
C	-7.788198000	-1.220483000	1.571973000
H	-8.812562000	-1.219253000	1.214103000
H	-7.538550000	-2.229307000	1.892110000
H	-7.730743000	-0.573848000	2.444698000
C	-6.937217000	0.500220000	-3.115145000
H	-7.510509000	-0.302270000	-3.573249000
H	-7.593159000	1.363006000	-3.022477000
H	-6.122400000	0.761545000	-3.782297000
C	7.797302000	4.170023000	-1.223864000
H	8.713069000	4.000828000	-0.661430000
H	8.058753000	4.190773000	-2.279622000
H	7.408368000	5.146039000	-0.951458000
C	6.458775000	-0.754148000	-1.301129000

H	6.411215000	-1.367591000	-0.404941000
H	5.749484000	-1.167300000	-2.014604000
H	7.455896000	-0.837972000	-1.721907000

TS1^F_{re}, $E_{(\text{SCF Done})} = -2955.34922494$ a.u. IF = $i224.33 \text{ cm}^{-1}$

Y	-1.907634000	0.311840000	0.217429000
N	-2.134037000	-2.296035000	-0.264406000
C	-2.172570000	-2.616321000	-1.701669000
H	-3.220060000	-2.619785000	-2.017883000
H	-1.767578000	-3.622636000	-1.897669000
C	-1.399250000	-1.595977000	-2.518567000
H	-0.350855000	-1.572462000	-2.224888000
H	-1.453617000	-1.840311000	-3.588507000
O	-1.903482000	-0.273293000	-2.306766000
C	-3.028279000	0.036097000	-3.128267000
H	-3.245927000	1.094287000	-2.982947000
H	-3.908783000	-0.554466000	-2.853718000
H	-2.773692000	-0.137151000	-4.181660000
O	0.134159000	-0.380553000	0.251402000
C	0.932429000	-1.396645000	-0.002544000
C	0.400748000	-2.707490000	-0.066921000
C	-1.002108000	-2.980418000	0.410141000
H	-1.175983000	-4.069948000	0.360089000
H	-1.081030000	-2.707828000	1.470612000
C	2.335208000	-1.224518000	-0.205678000
C	3.093882000	-2.343872000	-0.547769000
H	4.157460000	-2.210480000	-0.688357000
C	2.566676000	-3.636500000	-0.700174000
C	1.208127000	-3.788234000	-0.429390000
H	0.742506000	-4.768101000	-0.470466000
C	2.974715000	0.192581000	0.081439000
C	3.509375000	-4.815609000	-1.114171000
C	2.736518000	-6.153158000	-1.253208000
H	3.419408000	-6.939522000	-1.559552000
H	1.953495000	-6.078123000	-2.000725000
H	2.287647000	-6.448047000	-0.310470000
C	4.616476000	-5.004211000	-0.039187000
H	5.271948000	-5.825603000	-0.313325000
H	4.174889000	-5.228584000	0.927016000
H	5.220753000	-4.109139000	0.062349000
O	-4.021719000	-0.015581000	0.005806000
C	-4.937699000	-0.910477000	-0.313980000
C	-4.675978000	-2.291689000	-0.179186000
C	-3.378602000	-2.747398000	0.427114000

H	-3.300042000	-2.381125000	1.460824000
H	-3.380532000	-3.849807000	0.482397000
C	-6.205579000	-0.500468000	-0.803755000
C	-7.148010000	-1.464313000	-1.153321000
H	-8.115504000	-1.134158000	-1.525662000
C	-6.896411000	-2.839582000	-1.037672000
C	-5.649798000	-3.226424000	-0.546426000
H	-5.425027000	-4.285964000	-0.433950000
C	4.172635000	-4.496151000	-2.483504000
H	3.416715000	-4.362087000	-3.251342000
H	4.767117000	-3.590549000	-2.429406000
H	4.824229000	-5.310665000	-2.785809000
C	-1.890529000	2.593749000	-0.832788000
H	-1.093781000	2.125257000	-1.440506000
H	-2.872041000	2.235423000	-1.192905000
Si	-1.858568000	4.424296000	-1.266296000
C	-3.442435000	5.287102000	-0.652818000
H	-4.332873000	4.791729000	-1.058582000
H	-3.535871000	5.290838000	0.439129000
H	-3.461442000	6.331114000	-0.987745000
C	-1.792417000	4.662676000	-3.155955000
H	-2.656596000	4.198238000	-3.646067000
H	-1.791635000	5.727684000	-3.419917000
H	-0.886282000	4.212019000	-3.576770000
C	-0.335466000	5.294300000	-0.531036000
H	-0.360357000	5.327153000	0.563646000
H	0.582950000	4.776201000	-0.830050000
H	-0.270411000	6.327930000	-0.891140000
N	-1.886644000	0.113605000	2.637890000
C	-2.883212000	0.981956000	2.970206000
C	-1.572763000	-0.888880000	3.477808000
C	-3.715462000	0.705653000	4.083989000
C	-3.010887000	2.170829000	2.182974000
C	-2.286693000	-1.157797000	4.630092000
H	-0.717757000	-1.492760000	3.185357000
C	-3.410990000	-0.357394000	4.906886000
H	-4.553588000	1.362345000	4.297363000
H	-3.967458000	2.685185000	2.218238000
C	-1.963286000	2.760420000	1.476094000
H	-1.999505000	-1.978203000	5.279036000
H	-4.025740000	-0.563175000	5.779659000
H	-0.942190000	2.422043000	1.653464000
H	-2.039241000	3.815489000	1.263673000
C	2.453425000	0.634368000	1.490648000

C	1. 981311000	1. 909847000	1. 784179000
C	2. 490267000	-0. 299272000	2. 530350000
C	1. 574777000	2. 255733000	3. 072007000
H	1. 925685000	2. 659462000	1. 010810000
C	2. 084850000	0. 018752000	3. 817720000
H	2. 851665000	-1. 297796000	2. 328825000
C	1. 630279000	1. 305868000	4. 081169000
H	1. 318729000	1. 569837000	5. 083214000
C	2. 628964000	1. 223372000	-1. 039992000
C	3. 232234000	2. 489603000	-1. 015662000
C	1. 837385000	0. 906434000	-2. 129691000
C	3. 025052000	3. 413241000	-2. 021311000
H	3. 895700000	2. 742853000	-0. 200919000
C	1. 612535000	1. 822997000	-3. 163154000
H	1. 410086000	-0. 080639000	-2. 213287000
C	2. 201520000	3. 069853000	-3. 096554000
H	2. 040538000	3. 784996000	-3. 892294000
C	4. 541156000	0. 104251000	0. 088555000
C	5. 310566000	0. 213221000	1. 232212000
C	5. 209503000	-0. 064328000	-1. 133816000
C	6. 707397000	0. 146913000	1. 184540000
H	4. 840813000	0. 360482000	2. 192161000
C	6. 586128000	-0. 135594000	-1. 208344000
H	4. 630914000	-0. 137977000	-2. 043844000
C	7. 333402000	-0. 029711000	-0. 032313000
H	8. 412988000	-0. 081619000	-0. 081126000
C	2. 168859000	-1. 016403000	4. 938373000
H	3. 078752000	-0. 879651000	5. 520028000
H	1. 325975000	-0. 922907000	5. 617113000
H	2. 178671000	-2. 024448000	4. 535791000
C	1. 105344000	3. 676088000	3. 385817000
H	0. 993264000	4. 257379000	2. 476884000
H	0. 152282000	3. 665258000	3. 908172000
H	1. 825345000	4. 183313000	4. 024779000
C	3. 704128000	4. 781155000	-1. 986054000
H	2. 976962000	5. 577759000	-2. 121728000
H	4. 211714000	4. 937228000	-1. 039814000
H	4. 439143000	4. 865403000	-2. 783798000
C	0. 742027000	1. 422970000	-4. 352743000
H	-0. 277683000	1. 224758000	-4. 032286000
H	0. 718164000	2. 211312000	-5. 097902000
H	1. 124195000	0. 519565000	-4. 822337000
C	7. 512572000	0. 272758000	2. 476663000
H	8. 577734000	0. 224822000	2. 275350000

H	7.300148000	1.216809000	2.972924000
H	7.259305000	-0.527609000	3.168223000
C	7.294392000	-0.325117000	-2.548290000
H	7.987836000	0.491157000	-2.736445000
H	7.865167000	-1.251053000	-2.555231000
H	6.578697000	-0.359635000	-3.363094000
C	-7.964533000	-3.869174000	-1.432439000
H	-8.863837000	-3.746741000	-0.832639000
H	-8.247872000	-3.757275000	-2.476810000
H	-7.596008000	-4.879738000	-1.287519000
C	-6.495931000	0.998431000	-0.924643000
H	-6.319501000	1.501642000	0.023124000
H	-5.847753000	1.464196000	-1.664488000
H	-7.526598000	1.168558000	-1.220113000

P1^F_r, $E_{\text{(SCF Done)}} = -2955.37593019$ a.u.

Y	-1.920548000	-0.328285000	0.349691000
N	-1.766297000	-2.997105000	0.064589000
C	-1.775396000	-3.347252000	-1.366315000
H	-2.806220000	-3.585607000	-1.647989000
H	-1.164549000	-4.241582000	-1.568902000
C	-1.265616000	-2.199724000	-2.224474000
H	-0.230340000	-1.962352000	-1.979663000
H	-1.323537000	-2.452461000	-3.291241000
O	-2.010397000	-0.991922000	-1.989743000
C	-3.232219000	-0.897103000	-2.728221000
H	-3.646288000	0.087550000	-2.510621000
H	-3.946837000	-1.668137000	-2.420865000
H	-3.018850000	-0.983648000	-3.800427000
O	0.204459000	-0.738701000	0.488604000
C	1.147644000	-1.629069000	0.239419000
C	0.806997000	-3.001704000	0.207941000
C	-0.523059000	-3.439562000	0.750599000
H	-0.529419000	-4.542249000	0.801880000
H	-0.613431000	-3.079379000	1.786600000
C	2.511618000	-1.271560000	0.014294000
C	3.407491000	-2.284377000	-0.331472000
H	4.439052000	-2.008436000	-0.497885000
C	3.063029000	-3.639162000	-0.456623000
C	1.744590000	-3.971598000	-0.152621000
H	1.417564000	-5.006707000	-0.159008000
C	2.967694000	0.226403000	0.227690000
C	4.151467000	-4.683162000	-0.875023000
C	3.568274000	-6.116709000	-0.976866000

H	4.346653000	-6.806376000	-1.288316000
H	2.766382000	-6.163337000	-1.706500000
H	3.185119000	-6.454348000	-0.019586000
C	5.295879000	-4.697589000	0.176945000
H	6.052729000	-5.425490000	-0.100162000
H	4.909579000	-4.963383000	1.156221000
H	5.772390000	-3.725979000	0.251163000
O	-3.876519000	-1.066027000	0.831250000
C	-4.710584000	-2.008651000	0.422230000
C	-4.267083000	-3.342479000	0.308574000
C	-2.885186000	-3.672816000	0.783218000
H	-2.784517000	-3.378323000	1.836941000
H	-2.732264000	-4.765031000	0.740548000
C	-6.056610000	-1.707094000	0.090470000
C	-6.887733000	-2.728282000	-0.366201000
H	-7.917324000	-2.483687000	-0.618800000
C	-6.452962000	-4.055088000	-0.503673000
C	-5.132659000	-4.338253000	-0.153822000
H	-4.765194000	-5.360936000	-0.224534000
C	4.734852000	-4.298297000	-2.263747000
H	3.951851000	-4.283913000	-3.015880000
H	5.198509000	-3.318126000	-2.236231000
H	5.487030000	-5.019571000	-2.569270000
C	-1.459579000	3.556890000	-1.946101000
H	-0.443830000	3.759453000	-2.316217000
H	-2.015033000	3.177001000	-2.817385000
Si	-2.204356000	5.256284000	-1.478077000
C	-4.102843000	5.270317000	-1.573716000
H	-4.452560000	4.916343000	-2.550919000
H	-4.547231000	4.632300000	-0.803272000
H	-4.488404000	6.287026000	-1.431036000
C	-1.551648000	6.512649000	-2.750081000
H	-1.831579000	6.225329000	-3.770805000
H	-1.959819000	7.513017000	-2.563166000
H	-0.458321000	6.585651000	-2.712961000
C	-1.654892000	5.782200000	0.259651000
H	-2.061344000	5.105747000	1.019589000
H	-0.562477000	5.777771000	0.351056000
H	-2.005561000	6.795203000	0.490044000
N	-2.225145000	1.510943000	1.854488000
C	-3.125617000	2.051245000	0.961976000
C	-2.475245000	1.559620000	3.179008000
C	-4.370714000	2.534345000	1.456480000
C	-2.753126000	1.950642000	-0.414508000

C	-3.629449000	2.093593000	3.711844000
H	-1.702075000	1.134678000	3.816658000
C	-4.606322000	2.566763000	2.811256000
H	-5.107259000	2.909462000	0.752205000
H	-3.560692000	2.186654000	-1.109783000
C	-1.380449000	2.453546000	-0.872721000
H	-3.783671000	2.123666000	4.785204000
H	-5.541519000	2.973242000	3.189976000
H	-0.745398000	1.656887000	-1.300703000
H	-0.821140000	2.818897000	-0.002160000
C	2.333596000	0.708996000	1.574992000
C	1.759593000	1.955867000	1.759135000
C	2.383059000	-0.156234000	2.679310000
C	1.255189000	2.351190000	3.003341000
H	1.693289000	2.652914000	0.939192000
C	1.884346000	0.207594000	3.914998000
H	2.829915000	-1.133252000	2.562426000
C	1.321617000	1.476010000	4.069784000
H	0.939851000	1.775223000	5.036861000
C	2.556036000	1.115096000	-0.989461000
C	3.023576000	2.434538000	-1.070300000
C	1.832931000	0.620495000	-2.061297000
C	2.757582000	3.234748000	-2.164830000
H	3.632007000	2.829695000	-0.269230000
C	1.551876000	1.407787000	-3.182456000
H	1.507176000	-0.408171000	-2.058551000
C	2.012584000	2.709183000	-3.222858000
H	1.809669000	3.325394000	-4.088696000
C	4.532655000	0.321655000	0.311990000
C	5.221270000	0.522812000	1.494616000
C	5.283861000	0.216539000	-0.868527000
C	6.616983000	0.611692000	1.524750000
H	4.685504000	0.623543000	2.425475000
C	6.662305000	0.298116000	-0.866396000
H	4.771198000	0.070517000	-1.808587000
C	7.326232000	0.496540000	0.346493000
H	8.405959000	0.564833000	0.357691000
C	1.954368000	-0.748219000	5.104622000
H	2.548961000	-0.320973000	5.909080000
H	0.960643000	-0.946779000	5.499175000
H	2.401458000	-1.693713000	4.815716000
C	0.654529000	3.746240000	3.167045000
H	-0.212632000	3.869999000	2.523902000
H	0.345521000	3.916030000	4.193214000

H	1.378851000	4.511253000	2.897243000
C	3.268560000	4.672699000	-2.229592000
H	2.445502000	5.377607000	-2.130343000
H	3.978473000	4.867468000	-1.432369000
H	3.757020000	4.867065000	-3.180891000
C	0.746376000	0.820990000	-4.340108000
H	-0.298773000	0.705926000	-4.059769000
H	0.792396000	1.466974000	-5.210859000
H	1.126122000	-0.158800000	-4.618127000
C	7.329475000	0.836198000	2.857275000
H	8.403296000	0.901909000	2.715868000
H	6.988937000	1.756415000	3.326185000
H	7.124799000	0.019778000	3.546110000
C	7.460621000	0.176387000	-2.162932000
H	8.068759000	1.063082000	-2.325783000
H	8.130008000	-0.680144000	-2.124774000
H	6.799656000	0.054823000	-3.014804000
C	-7.409319000	-5.147022000	-1.003378000
H	-8.256463000	-5.259827000	-0.330204000
H	-7.801631000	-4.902048000	-1.987980000
H	-6.899750000	-6.103095000	-1.069091000
C	-6.556737000	-0.268213000	0.237529000
H	-6.327200000	0.119110000	1.226722000
H	-6.078471000	0.387217000	-0.488098000
H	-7.630370000	-0.217535000	0.085302000

C2^F_{sym}, $E_{(\text{SCF Done})} = -3280.91098211 \text{ a.u.}$

Y	-1.531139000	-0.567787000	0.259787000
N	-0.960271000	-2.946725000	-0.733102000
C	-0.949365000	-2.917037000	-2.206452000
H	-1.955163000	-3.172789000	-2.554143000
H	-0.259964000	-3.671525000	-2.618618000
C	-0.561758000	-1.546653000	-2.742550000
H	0.445039000	-1.268777000	-2.435927000
H	-0.601742000	-1.542498000	-3.839840000
O	-1.432341000	-0.521687000	-2.238764000
C	-2.612370000	-0.361383000	-3.030791000
H	-3.179412000	0.462170000	-2.602301000
H	-3.228778000	-1.266196000	-3.017836000
H	-2.325897000	-0.113312000	-4.059903000
O	0.669897000	-0.604709000	0.232201000
C	1.699687000	-1.234945000	-0.317348000
C	1.566711000	-2.611981000	-0.631063000
C	0.349488000	-3.368309000	-0.177110000

H	0.500969000	-4.436451000	-0.411420000
H	0.254327000	-3.300628000	0.914336000
C	2.947436000	-0.606406000	-0.624442000
C	3.933338000	-1.374567000	-1.255816000
H	4.880138000	-0.894640000	-1.461384000
C	3.787502000	-2.716057000	-1.627621000
C	2.579542000	-3.317396000	-1.280916000
H	2.401657000	-4.366851000	-1.492830000
C	3.330958000	0.814433000	-0.046745000
C	4.956031000	-3.457901000	-2.358015000
C	6.219879000	-3.465208000	-1.452940000
H	7.032583000	-3.990841000	-1.945516000
H	6.011727000	-3.964592000	-0.511556000
H	6.553072000	-2.455835000	-1.236990000
O	-3.435440000	-1.453015000	-0.160452000
C	-4.056317000	-2.528894000	-0.621419000
C	-3.372233000	-3.761368000	-0.732345000
C	-1.970611000	-3.906264000	-0.209970000
H	-1.962051000	-3.785877000	0.882129000
H	-1.628051000	-4.936212000	-0.410878000
C	-5.421716000	-2.481429000	-1.009215000
C	-6.031231000	-3.628080000	-1.517123000
H	-7.078661000	-3.569821000	-1.805088000
C	-5.353983000	-4.845296000	-1.662072000
C	-4.020204000	-4.883415000	-1.258692000
H	-3.463894000	-5.816072000	-1.338148000
C	5.283381000	-2.727904000	-3.690943000
H	4.414640000	-2.715169000	-4.342167000
H	5.589336000	-1.702851000	-3.511356000
H	6.090574000	-3.235886000	-4.210314000
C	-5.284595000	2.931041000	-1.541442000
H	-5.211497000	2.725093000	-2.620357000
H	-6.299874000	2.618371000	-1.252762000
Si	-5.185467000	4.830176000	-1.328282000
C	-5.977006000	5.420536000	0.295089000
H	-7.001994000	5.044628000	0.399106000
H	-5.399148000	5.075875000	1.158661000
H	-6.019095000	6.516189000	0.327485000
C	-6.151858000	5.607699000	-2.774207000
H	-7.196730000	5.274198000	-2.778039000
H	-6.153129000	6.702132000	-2.706015000
H	-5.711466000	5.334009000	-3.740589000
C	-3.383357000	5.418557000	-1.392507000
H	-2.805363000	4.954161000	-0.585780000

H	-2.908617000	5.162423000	-2.346971000
H	-3.322222000	6.506479000	-1.270811000
N	-2.038190000	1.523523000	1.185748000
C	-3.277229000	2.095314000	1.573508000
C	-0.947146000	1.840426000	1.953982000
C	-3.390502000	2.525702000	2.961276000
C	-4.314783000	2.258237000	0.703131000
C	-0.990550000	2.455162000	3.174329000
H	0.005796000	1.523172000	1.535317000
C	-2.285054000	2.730342000	3.722205000
H	-4.383321000	2.760052000	3.339141000
C	-4.254572000	2.075152000	-0.780907000
H	-0.080918000	2.671340000	3.722399000
H	-2.378834000	3.109311000	4.738011000
H	-4.411549000	1.022744000	-1.061625000
H	-3.237562000	2.326865000	-1.123800000
C	3.664292000	0.510809000	1.451239000
C	2.855181000	0.861412000	2.516893000
C	4.815740000	-0.242267000	1.728688000
C	3.186480000	0.514738000	3.832478000
H	1.951588000	1.423681000	2.350570000
C	5.160863000	-0.603862000	3.014770000
H	5.454091000	-0.547786000	0.912814000
C	4.335101000	-0.211492000	4.071034000
H	4.600620000	-0.483243000	5.084004000
C	2.235780000	1.898306000	-0.282415000
C	2.225789000	3.075032000	0.457409000
C	1.381883000	1.809697000	-1.384498000
C	1.350054000	4.115737000	0.159493000
H	2.923050000	3.202470000	1.272107000
C	0.514460000	2.842570000	-1.715741000
H	1.429385000	0.940094000	-2.022996000
C	0.496029000	3.988736000	-0.924647000
H	-0.174663000	4.799088000	-1.176674000
C	4.561379000	1.452890000	-0.778096000
C	5.558479000	2.122503000	-0.088345000
C	4.601648000	1.481161000	-2.177502000
C	6.597992000	2.774694000	-0.755848000
H	5.542834000	2.152430000	0.990905000
C	5.619711000	2.117773000	-2.862089000
H	3.818217000	0.993717000	-2.739219000
C	6.624293000	2.761112000	-2.137162000
H	7.424737000	3.261742000	-2.665526000
C	6.425434000	-1.413884000	3.293495000

H	7.124951000	-0.840114000	3.897502000
H	6.188777000	-2.324296000	3.838973000
H	6.920906000	-1.688856000	2.368191000
C	2.289899000	0.961906000	4.985833000
H	1.249649000	0.717000000	4.789846000
H	2.587669000	0.484899000	5.913990000
H	2.353333000	2.039169000	5.124138000
C	1.331502000	5.375436000	1.022681000
H	0.979008000	6.230093000	0.453679000
H	0.666073000	5.241578000	1.873872000
H	2.323193000	5.598263000	1.405119000
C	-0.363245000	2.759852000	-2.963158000
H	-1.408951000	2.914278000	-2.713428000
H	-0.077714000	3.525883000	-3.681281000
H	-0.262966000	1.791568000	-3.441276000
C	7.681228000	3.491594000	0.048059000
H	8.401716000	3.965841000	-0.610240000
H	7.244670000	4.256790000	0.685621000
H	8.212736000	2.791854000	0.689031000
C	5.654715000	2.128012000	-4.389178000
H	6.552224000	1.636242000	-4.757727000
H	4.791749000	1.614328000	-4.799903000
H	5.658116000	3.147480000	-4.767613000
C	-2.142092000	-2.343772000	3.408677000
C	-1.701713000	-3.132713000	4.482355000
C	-0.361212000	-3.144531000	4.837671000
C	0.525313000	-2.361768000	4.103042000
C	0.031026000	-1.644178000	3.020879000
N	-1.263869000	-1.642573000	2.646938000
H	-0.017509000	-3.742018000	5.677899000
H	-2.433081000	-3.703748000	5.046561000
H	1.583815000	-2.317001000	4.338265000
H	0.699839000	-1.066717000	2.390807000
C	-3.583491000	-2.266636000	3.149781000
H	-4.153984000	-3.161641000	3.394258000
C	-4.215089000	-1.165104000	2.734070000
H	-5.256879000	2.609701000	1.120305000
C	4.589063000	-4.928062000	-2.688820000
H	4.386645000	-5.495247000	-1.786261000
H	3.717256000	-4.979774000	-3.332847000
H	5.416907000	-5.403851000	-3.205350000
C	-6.217069000	-1.179509000	-0.869890000
H	-5.887402000	-0.617453000	-0.001950000
H	-6.087938000	-0.544262000	-1.743968000

H	-7.277081000	-1.391106000	-0.767128000
C	-6.060621000	-6.078437000	-2.241681000
H	-5.421939000	-6.953586000	-2.175902000
H	-6.982060000	-6.287227000	-1.703322000
H	-6.317806000	-5.924978000	-3.287915000
H	-5.290378000	-1.160731000	2.587404000
H	-3.695864000	-0.229218000	2.552273000

TS2^F_{syn}, $E_{(\text{SCF Done})} = -3280.89540336 \text{ a.u.}$ IF = $i166.00 \text{ cm}^{-1}$

Y	1.508698000	0.544148000	0.263564000
N	0.907641000	3.030366000	-0.086892000
C	0.874551000	3.356922000	-1.526043000
H	1.884529000	3.641209000	-1.831971000
H	0.219628000	4.221365000	-1.722362000
C	0.397256000	2.184454000	-2.374631000
H	-0.626899000	1.910021000	-2.131115000
H	0.440034000	2.454576000	-3.437774000
O	1.190916000	1.006541000	-2.158147000
C	2.296155000	0.888794000	-3.055128000
H	2.817357000	-0.034930000	-2.800941000
H	2.984784000	1.732847000	-2.952602000
H	1.924950000	0.825366000	-4.084863000
O	-0.682356000	0.539042000	0.204973000
C	-1.748938000	1.294217000	-0.041190000
C	-1.625483000	2.704838000	0.034049000
C	-0.377131000	3.340095000	0.579746000
H	-0.517896000	4.434470000	0.568592000
H	-0.244800000	3.065754000	1.634760000
C	-3.038129000	0.766712000	-0.376591000
C	-4.069834000	1.669570000	-0.651061000
H	-5.046358000	1.259715000	-0.863484000
C	-3.936022000	3.063338000	-0.652733000
C	-2.686334000	3.553574000	-0.288246000
H	-2.508878000	4.622002000	-0.220143000
C	-3.359221000	-0.771068000	-0.200705000
C	-5.161008000	3.967559000	-1.013594000
C	-6.311232000	3.720126000	0.002381000
H	-7.163200000	4.351048000	-0.233066000
H	-5.984482000	3.951305000	1.011696000
H	-6.639736000	2.686617000	-0.021413000
O	3.365402000	1.553645000	-0.246661000
C	3.923357000	2.738430000	-0.478743000
C	3.276412000	3.910198000	-0.022384000
C	1.953913000	3.790335000	0.668018000

H	2.057025000	3.281481000	1.638622000
H	1.576748000	4.802438000	0.886249000
C	5.131671000	2.893099000	-1.208163000
C	5.664453000	4.173251000	-1.385194000
H	6.594270000	4.265151000	-1.942075000
C	5.053876000	5.330361000	-0.894036000
C	3.839957000	5.170235000	-0.225762000
H	3.309029000	6.046791000	0.141290000
C	-5.657398000	3.623445000	-2.445984000
H	-4.869113000	3.791499000	-3.173540000
H	-5.968805000	2.586678000	-2.514361000
H	-6.504357000	4.249261000	-2.711127000
C	6.303680000	-2.141267000	-0.619139000
H	6.870753000	-1.570368000	-1.371309000
H	7.011280000	-2.314969000	0.206110000
Si	5.896595000	-3.826742000	-1.420411000
C	5.468753000	-5.164260000	-0.142858000
H	6.272085000	-5.269572000	0.596254000
H	4.544293000	-4.924578000	0.392608000
H	5.336272000	-6.137317000	-0.631622000
C	7.445269000	-4.391476000	-2.373665000
H	8.307735000	-4.493497000	-1.704024000
H	7.280326000	-5.363719000	-2.853270000
H	7.715331000	-3.673709000	-3.157445000
C	4.459724000	-3.627723000	-2.648444000
H	3.544943000	-3.317458000	-2.131271000
H	4.695527000	-2.874420000	-3.410400000
H	4.251939000	-4.571948000	-3.165520000
N	2.134236000	-1.807335000	0.196071000
C	3.110017000	-2.322828000	1.059268000
C	1.016643000	-2.556459000	-0.000015000
C	2.726823000	-3.386157000	1.947544000
C	4.424087000	-1.853959000	1.071695000
C	0.711824000	-3.712266000	0.680426000
H	0.319327000	-2.162335000	-0.733821000
C	1.574387000	-4.090941000	1.738243000
H	3.429803000	-3.678925000	2.722729000
C	5.130350000	-1.273417000	-0.117632000
H	-0.187749000	-4.268840000	0.449988000
H	1.331505000	-4.944172000	2.367423000
H	5.522478000	-0.273114000	0.109900000
H	4.405537000	-1.124462000	-0.926973000
C	-3.207517000	-1.011180000	1.335282000
C	-2.267021000	-1.845868000	1.909904000

C	-4.055996000	-0.289663000	2.190177000
C	-2.185776000	-2.000355000	3.300538000
H	-1.578113000	-2.399838000	1.292007000
C	-3.996572000	-0.425808000	3.561305000
H	-4.781960000	0.386065000	1.761037000
C	-3.054156000	-1.298632000	4.111180000
H	-3.002129000	-1.417328000	5.185239000
C	-2.485971000	-1.693610000	-1.104298000
C	-2.571414000	-3.079969000	-0.956237000
C	-1.789384000	-1.195346000	-2.199226000
C	-1.956520000	-3.945615000	-1.847343000
H	-3.153480000	-3.491461000	-0.144110000
C	-1.165539000	-2.045227000	-3.111391000
H	-1.763245000	-0.130592000	-2.374239000
C	-1.248766000	-3.415967000	-2.922427000
H	-0.772896000	-4.083304000	-3.628849000
C	-4.807465000	-1.135132000	-0.684761000
C	-5.718993000	-1.815467000	0.101866000
C	-5.163302000	-0.869175000	-2.015596000
C	-6.970790000	-2.197971000	-0.392399000
H	-5.473465000	-2.070974000	1.121183000
C	-6.392512000	-1.233225000	-2.527153000
H	-4.455017000	-0.367460000	-2.659377000
C	-7.300224000	-1.898414000	-1.698449000
H	-8.265471000	-2.188866000	-2.091483000
C	-4.946775000	0.348743000	4.472536000
H	-5.639150000	-0.327104000	4.970160000
H	-4.396644000	0.881901000	5.243942000
H	-5.526210000	1.069553000	3.904927000
C	-1.147448000	-2.945929000	3.900609000
H	-0.142204000	-2.651915000	3.609020000
H	-1.205397000	-2.944393000	4.984140000
H	-1.306319000	-3.963319000	3.551282000
C	-2.073938000	-5.459593000	-1.680343000
H	-2.637417000	-5.893397000	-2.503614000
H	-1.090986000	-5.924018000	-1.671180000
H	-2.580253000	-5.709140000	-0.753700000
C	-0.419882000	-1.485389000	-4.321235000
H	0.645042000	-1.694005000	-4.248159000
H	-0.782246000	-1.939253000	-5.240397000
H	-0.553832000	-0.411370000	-4.395065000
C	-7.946369000	-2.940812000	0.518659000
H	-8.857189000	-3.193884000	-0.014006000
H	-7.501150000	-3.860132000	0.891741000

H	-8.211924000	-2.330235000	1.378720000
C	-6.766368000	-0.924780000	-3.975647000
H	-7.632809000	-0.268551000	-4.018899000
H	-5.945128000	-0.439511000	-4.492732000
H	-7.016681000	-1.837302000	-4.511513000
C	2.324324000	0.437285000	3.827287000
C	1.899766000	0.534425000	5.179856000
C	0.605813000	0.864529000	5.508203000
C	-0.313283000	1.074533000	4.471477000
C	0.141571000	0.942706000	3.173338000
N	1.418040000	0.661778000	2.815481000
H	0.304354000	0.946400000	6.549519000
H	2.635896000	0.350226000	5.956743000
H	-1.356810000	1.302936000	4.658149000
H	-0.561521000	1.029499000	2.352505000
C	3.698302000	0.099215000	3.604091000
H	4.222510000	-0.222743000	4.502127000
C	4.393754000	0.100824000	2.427115000
H	5.067321000	-2.371116000	1.782841000
C	-4.796381000	5.474528000	-0.976437000
H	-4.480219000	5.778225000	0.016068000
H	-4.000997000	5.703299000	-1.678271000
H	-5.664643000	6.066995000	-1.247663000
C	5.872622000	1.695692000	-1.813440000
H	6.656275000	1.341162000	-1.147846000
H	5.195167000	0.870747000	-1.997438000
H	6.339703000	1.977997000	-2.752720000
C	5.696574000	6.711470000	-1.079275000
H	4.953181000	7.498103000	-0.992378000
H	6.460688000	6.888080000	-0.324100000
H	6.169862000	6.791621000	-2.053989000
H	5.466446000	-0.062225000	2.459764000
H	4.050415000	0.623210000	1.540513000

P2^F_{syn}, $E_{(\text{SCF Done})} = -3280.95059466 \text{ a.u.}$

Y	1.303272000	0.687501000	0.486694000
N	0.585573000	3.145437000	-0.024167000
C	0.401654000	3.448693000	-1.454560000
H	1.333128000	3.887046000	-1.824550000
H	-0.395072000	4.194638000	-1.605343000
C	0.068717000	2.206152000	-2.261400000
H	-0.888789000	1.797973000	-1.952077000
H	0.017787000	2.449875000	-3.331700000
O	1.028285000	1.163508000	-2.054884000

C	2.175839000	1.269513000	-2.894491000
H	2.821834000	0.424042000	-2.656277000
H	2.728596000	2.196392000	-2.713182000
H	1.869185000	1.215997000	-3.947667000
O	-0.874764000	0.522673000	0.345663000
C	-1.978088000	1.227775000	0.180578000
C	-1.916816000	2.643782000	0.282251000
C	-0.663048000	3.328358000	0.763573000
H	-0.873747000	4.409801000	0.834466000
H	-0.433474000	2.989925000	1.783138000
C	-3.251801000	0.636730000	-0.110183000
C	-4.346677000	1.486719000	-0.287094000
H	-5.309308000	1.033870000	-0.473178000
C	-4.289693000	2.885513000	-0.226694000
C	-3.044916000	3.436571000	0.065503000
H	-2.924474000	4.511499000	0.157202000
C	-3.419123000	-0.938862000	-0.152968000
C	-5.587098000	3.729697000	-0.458430000
C	-6.648991000	3.362321000	0.615886000
H	-7.551418000	3.948729000	0.470020000
H	-6.268159000	3.564829000	1.612281000
H	-6.915614000	2.312351000	0.560410000
O	3.185241000	1.713559000	0.023696000
C	3.679415000	2.883535000	-0.326287000
C	2.944485000	4.078461000	-0.139563000
C	1.619175000	4.041133000	0.567720000
H	1.766382000	3.697793000	1.596210000
H	1.216555000	5.067527000	0.625547000
C	4.971892000	2.980768000	-0.912152000
C	5.467155000	4.222808000	-1.300333000
H	6.458930000	4.269776000	-1.745578000
C	4.738395000	5.409092000	-1.133753000
C	3.477598000	5.305803000	-0.547882000
H	2.886018000	6.206919000	-0.391785000
C	-6.161534000	3.429007000	-1.871491000
H	-5.436044000	3.679828000	-2.639439000
H	-6.418267000	2.380284000	-1.975246000
H	-7.058721000	4.015411000	-2.046504000
C	5.878641000	-3.249894000	0.104065000
H	5.865744000	-4.000228000	0.909924000
H	5.341770000	-3.703780000	-0.740969000
Si	7.697808000	-3.038272000	-0.441813000
C	7.794821000	-1.967984000	-2.006845000
H	7.206843000	-2.404997000	-2.822604000

H	7.416780000	-0.956052000	-1.824153000
H	8.830935000	-1.877846000	-2.353744000
C	8.398091000	-4.763610000	-0.819800000
H	7.826539000	-5.259933000	-1.612985000
H	9.441197000	-4.699926000	-1.151166000
H	8.368951000	-5.407319000	0.067141000
C	8.714901000	-2.234416000	0.944967000
H	8.357785000	-1.223374000	1.171779000
H	8.664934000	-2.823328000	1.868394000
H	9.769794000	-2.155928000	0.656721000
N	2.019051000	-1.559390000	-0.576728000
C	2.764000000	-2.517402000	0.019540000
C	1.232204000	-1.910395000	-1.610058000
C	2.677096000	-3.851406000	-0.398062000
C	3.729276000	-2.155088000	1.124894000
C	1.128920000	-3.206543000	-2.098333000
H	0.651485000	-1.107319000	-2.053011000
C	1.861379000	-4.204361000	-1.465583000
H	3.253278000	-4.604970000	0.128936000
C	5.170417000	-1.976092000	0.574127000
H	0.469992000	-3.417215000	-2.933760000
H	1.796485000	-5.239112000	-1.791970000
H	5.753196000	-1.516284000	1.383766000
H	5.137913000	-1.234800000	-0.233924000
C	-2.754777000	-1.512367000	1.139724000
C	-1.887138000	-2.598434000	1.158122000
C	-3.104630000	-0.938559000	2.364719000
C	-1.422044000	-3.136265000	2.356444000
H	-1.563985000	-3.053141000	0.235564000
C	-2.658468000	-1.457793000	3.570755000
H	-3.762799000	-0.080816000	2.375585000
C	-1.826726000	-2.571914000	3.556418000
H	-1.485985000	-2.997902000	4.490438000
C	-2.838556000	-1.553539000	-1.467809000
C	-2.994493000	-2.926458000	-1.709554000
C	-2.311692000	-0.777550000	-2.485100000
C	-2.609664000	-3.504371000	-2.903919000
H	-3.457833000	-3.546166000	-0.955227000
C	-1.920395000	-1.334834000	-3.706354000
H	-2.244022000	0.290393000	-2.355580000
C	-2.064718000	-2.694609000	-3.902420000
H	-1.776131000	-3.135565000	-4.847371000
C	-4.939913000	-1.345781000	-0.191545000
C	-5.604916000	-1.945587000	0.862021000

C	-5.662699000	-1.136011000	-1.377503000
C	-6.950848000	-2.317404000	0.766284000
H	-5.089465000	-2.148386000	1.787118000
C	-6.991081000	-1.490210000	-1.497782000
H	-5.165374000	-0.685376000	-2.224325000
C	-7.634297000	-2.084394000	-0.408792000
H	-8.674713000	-2.368565000	-0.494386000
C	-3.109491000	-0.828699000	4.887809000
H	-4.171352000	-1.000300000	5.052683000
H	-2.565441000	-1.251934000	5.725813000
H	-2.946217000	0.245714000	4.878493000
C	-0.516826000	-4.367104000	2.342257000
H	0.089643000	-4.413294000	3.241293000
H	-1.109895000	-5.278950000	2.291751000
H	0.143759000	-4.351422000	1.480992000
C	-2.788899000	-5.001791000	-3.147085000
H	-3.355801000	-5.179757000	-4.057563000
H	-1.824812000	-5.493748000	-3.257602000
H	-3.314391000	-5.467646000	-2.319979000
C	-1.347580000	-0.445981000	-4.809081000
H	-1.491082000	-0.899443000	-5.784888000
H	-1.826479000	0.528762000	-4.808614000
H	-0.279600000	-0.292920000	-4.666618000
C	-7.636793000	-2.974504000	1.962727000
H	-8.660123000	-3.243815000	1.722542000
H	-7.107186000	-3.875067000	2.264343000
H	-7.652707000	-2.300047000	2.815940000
C	-7.757837000	-1.243821000	-2.795637000
H	-8.584690000	-0.556590000	-2.630365000
H	-7.108750000	-0.819307000	-3.554456000
H	-8.172830000	-2.172309000	-3.180578000
C	1.369630000	0.022080000	3.274809000
C	0.685395000	-0.281806000	4.485932000
C	0.315985000	0.729509000	5.342446000
C	0.601801000	2.066127000	5.005994000
C	1.195742000	2.303236000	3.782395000
N	1.541705000	1.335563000	2.913165000
H	-0.165098000	0.495737000	6.289512000
H	0.518063000	-1.323098000	4.741335000
H	0.358892000	2.888038000	5.671212000
H	1.404031000	3.324856000	3.471149000
C	1.849537000	-0.948321000	2.342540000
H	1.497812000	-1.960004000	2.554417000
C	3.324312000	-0.923676000	1.945353000

H	3.746411000	-3.018152000	1.807473000
C	-5.310170000	5.252849000	-0.364137000
H	-4.939486000	5.524591000	0.618704000
H	-4.583731000	5.566629000	-1.106643000
H	-6.229354000	5.803103000	-0.539963000
C	5.797442000	1.702611000	-1.083478000
H	5.980325000	1.231043000	-0.120814000
H	5.275274000	0.979482000	-1.706247000
H	6.755385000	1.921590000	-1.545090000
C	5.320839000	6.760659000	-1.570553000
H	4.604144000	7.558948000	-1.405366000
H	6.223828000	6.996244000	-1.011052000
H	5.581865000	6.752105000	-2.626610000
H	3.983221000	-0.911930000	2.831885000
H	3.622492000	-0.019565000	1.389727000

C2^F, $E_{(\text{SCF Done})} = -3280.91673744 \text{ a.u.}$

Y	1.743530000	-0.327107000	0.236531000
N	1.473109000	-2.696704000	-0.729613000
C	1.145985000	-3.704720000	0.297671000
H	2.085908000	-4.112856000	0.679734000
H	0.579698000	-4.542375000	-0.140776000
C	0.346362000	-3.109446000	1.442972000
H	-0.605684000	-2.719421000	1.091209000
H	0.150983000	-3.874509000	2.206745000
O	1.033792000	-2.003989000	2.039084000
C	1.928085000	-2.383099000	3.081354000
H	2.371933000	-1.465885000	3.469019000
H	2.724747000	-3.038568000	2.714380000
H	1.368268000	-2.884018000	3.882131000
O	-0.448761000	-0.452259000	-0.130741000
C	-1.375865000	-1.192679000	-0.715019000
C	-0.994163000	-2.361085000	-1.432596000
C	0.440473000	-2.646462000	-1.792220000
H	0.462745000	-3.611540000	-2.327533000
H	0.793898000	-1.898856000	-2.509962000
C	-2.780605000	-0.895376000	-0.661701000
C	-3.675060000	-1.792496000	-1.252121000
H	-4.726201000	-1.550768000	-1.212188000
C	-3.309740000	-2.977264000	-1.900359000
C	-1.943919000	-3.226753000	-1.979360000
H	-1.574221000	-4.104576000	-2.499986000
C	-3.326859000	0.415779000	0.043737000
C	-4.409267000	-3.913106000	-2.503109000

C	-5.214559000	-3.144047000	-3.587897000
H	-5.976659000	-3.786829000	-4.018722000
H	-4.557363000	-2.812405000	-4.385981000
H	-5.705252000	-2.272860000	-3.167306000
O	3.633477000	-1.342924000	0.672291000
C	4.306603000	-2.466248000	0.480293000
C	3.910420000	-3.368538000	-0.533099000
C	2.756629000	-3.022069000	-1.425075000
H	2.998935000	-2.151067000	-2.048854000
H	2.581302000	-3.863934000	-2.115734000
C	5.432019000	-2.814091000	1.277304000
C	6.102499000	-4.012763000	1.037037000
H	6.961780000	-4.255417000	1.658586000
C	5.716158000	-4.910196000	0.033496000
C	4.608188000	-4.562083000	-0.737171000
H	4.271746000	-5.233545000	-1.525569000
C	-5.377098000	-4.375420000	-1.377631000
H	-4.835891000	-4.917370000	-0.607977000
H	-5.871490000	-3.528687000	-0.913823000
H	-6.141113000	-5.032281000	-1.782982000
C	3.179671000	4.240078000	-0.134082000
H	2.452418000	5.012267000	0.162828000
H	3.920570000	4.210886000	0.679316000
Si	4.060549000	4.909030000	-1.693331000
C	5.750398000	4.094514000	-1.993046000
H	6.366651000	4.109400000	-1.086193000
H	5.633369000	3.053254000	-2.309382000
H	6.299874000	4.626375000	-2.779377000
C	4.349675000	6.769019000	-1.401462000
H	4.963366000	6.939964000	-0.508598000
H	4.867814000	7.226508000	-2.252725000
H	3.402227000	7.303008000	-1.261412000
C	2.977302000	4.684120000	-3.234744000
H	2.810635000	3.621225000	-3.441541000
H	1.998980000	5.162681000	-3.110609000
H	3.456615000	5.126516000	-4.116174000
N	2.015665000	0.582650000	-2.019468000
C	3.298100000	0.956489000	-1.648450000
C	1.807623000	0.118391000	-3.272363000
C	4.398367000	0.465630000	-2.428713000
C	3.392064000	1.712534000	-0.469242000
C	2.826285000	-0.179875000	-4.150632000
H	0.764590000	-0.033289000	-3.545888000
C	4.156816000	-0.063383000	-3.671239000

H	5.410698000	0.590884000	-2.054729000
C	2.453455000	2.879252000	-0.202719000
H	2.612688000	-0.537213000	-5.152505000
H	4.988553000	-0.372764000	-4.300454000
H	1.898120000	2.778870000	0.743203000
H	1.690466000	2.899696000	-0.989251000
C	-2.398512000	1.611558000	-0.344975000
C	-2.014175000	2.607017000	0.537435000
C	-2.002214000	1.739161000	-1.685032000
C	-1.280900000	3.718675000	0.112001000
H	-2.289239000	2.549262000	1.577834000
C	-1.281715000	2.830677000	-2.131941000
H	-2.288393000	0.973417000	-2.392094000
C	-0.930552000	3.828115000	-1.219438000
H	-0.379257000	4.693570000	-1.561838000
C	-3.434383000	0.210470000	1.590986000
C	-4.110933000	1.160365000	2.371850000
C	-2.983500000	-0.934595000	2.222532000
C	-4.316983000	0.978297000	3.725619000
H	-4.510690000	2.045576000	1.898085000
C	-3.177568000	-1.145226000	3.591573000
H	-2.497866000	-1.705235000	1.645193000
C	-3.840533000	-0.186823000	4.332333000
H	-4.005606000	-0.341981000	5.390255000
C	-4.792899000	0.732860000	-0.439165000
C	-5.092014000	1.699081000	-1.383312000
C	-5.867325000	0.015528000	0.111295000
C	-6.407322000	1.955374000	-1.784804000
H	-4.305705000	2.287186000	-1.828509000
C	-7.174593000	0.246365000	-0.268622000
H	-5.670972000	-0.741679000	0.856260000
C	-7.438101000	1.227535000	-1.226886000
H	-8.459490000	1.417833000	-1.528727000
C	-0.885410000	2.962575000	-3.600958000
H	0.193375000	2.890268000	-3.715292000
H	-1.343494000	2.179598000	-4.196308000
H	-1.197390000	3.924744000	-3.999854000
C	-0.902201000	4.803535000	1.119219000
H	-0.275200000	4.396921000	1.909070000
H	-0.358924000	5.608137000	0.634885000
H	-1.790033000	5.223947000	1.586258000
C	-5.068837000	2.017929000	4.554691000
H	-4.451965000	2.380087000	5.373954000
H	-5.356472000	2.866455000	3.942695000

H	-5.969565000	1.587306000	4.986099000
C	-2.656182000	-2.422895000	4.246591000
H	-1.575509000	-2.379216000	4.367861000
H	-3.098801000	-2.564162000	5.227372000
H	-2.886435000	-3.292020000	3.636360000
C	-6.678011000	3.035348000	-2.830808000
H	-7.742105000	3.134200000	-3.018822000
H	-6.298017000	3.998418000	-2.498095000
H	-6.186117000	2.793573000	-3.770248000
C	-8.324107000	-0.553547000	0.341254000
H	-8.840975000	-1.129559000	-0.423166000
H	-7.959472000	-1.241225000	1.097222000
H	-9.052265000	0.108684000	0.803566000
C	2.149460000	1.806141000	3.364350000
C	1.547083000	2.465377000	4.447556000
C	0.200733000	2.283958000	4.721445000
C	-0.533121000	1.448521000	3.887923000
C	0.119625000	0.841428000	2.820078000
N	1.425956000	0.998450000	2.543877000
H	-0.265542000	2.786838000	5.564481000
H	2.158933000	3.108339000	5.073127000
H	-1.590504000	1.270046000	4.041819000
H	-0.439471000	0.213817000	2.132412000
C	3.583095000	2.030565000	3.170567000
H	3.967656000	2.902709000	3.697710000
C	4.431003000	1.267554000	2.473577000
H	5.480778000	1.544026000	2.415254000
H	4.140894000	0.362296000	1.950372000
H	4.401949000	1.838008000	-0.081385000
C	-3.795330000	-5.176593000	-3.160653000
H	-3.137337000	-4.911763000	-3.981713000
H	-3.231261000	-5.759499000	-2.439846000
H	-4.587509000	-5.805440000	-3.555161000
C	5.919664000	-1.864787000	2.376447000
H	6.300851000	-0.940383000	1.949720000
H	5.115765000	-1.604092000	3.059928000
H	6.717270000	-2.326276000	2.950084000
C	6.493418000	-6.212230000	-0.204432000
H	7.493814000	-6.006031000	-0.579976000
H	6.598527000	-6.778665000	0.717944000
H	5.983312000	-6.836701000	-0.931101000

TS2_{iso}^F , $E_{(\text{SCF Done})} = -3280.90687878 \text{ a.u.}$ IF = $i89.26 \text{ cm}^{-1}$

Y	1.506697000	-0.686256000	0.289118000
N	1.032503000	-2.948249000	-0.957309000
C	0.591878000	-4.006756000	-0.028523000
H	1.481148000	-4.541515000	0.317916000
H	-0.051297000	-4.740636000	-0.540969000
C	-0.156601000	-3.440333000	1.165564000
H	-1.062740000	-2.929136000	0.847730000
H	-0.434693000	-4.246163000	1.857991000
O	0.627959000	-2.464497000	1.862071000
C	1.487546000	-3.015371000	2.859180000
H	1.993316000	-2.176036000	3.337427000
H	2.236402000	-3.684705000	2.422893000
H	0.888692000	-3.554272000	3.604124000
O	-0.579899000	-0.532923000	-0.253131000
C	-1.605094000	-1.131477000	-0.842184000
C	-1.369872000	-2.282711000	-1.635361000
C	0.027421000	-2.695873000	-2.021033000
H	-0.049074000	-3.605545000	-2.641309000
H	0.471324000	-1.928137000	-2.666610000
C	-2.953498000	-0.669591000	-0.714985000
C	-3.962513000	-1.409827000	-1.335922000
H	-4.976182000	-1.048003000	-1.249178000
C	-3.750876000	-2.581870000	-2.073802000
C	-2.427210000	-2.990150000	-2.211269000
H	-2.178225000	-3.867909000	-2.798938000
C	-3.286163000	0.655703000	0.086845000
C	-4.967796000	-3.334598000	-2.707946000
C	-5.694985000	-2.397889000	-3.713052000
H	-6.537083000	-2.912962000	-4.165811000
H	-5.018305000	-2.089756000	-4.504254000
H	-6.069066000	-1.507576000	-3.219082000
O	3.305350000	-1.853497000	0.486845000
C	3.874253000	-3.027402000	0.255485000
C	3.400678000	-3.842261000	-0.794565000
C	2.288760000	-3.343238000	-1.669299000
H	2.610809000	-2.458842000	-2.236475000
H	2.046125000	-4.123131000	-2.410607000
C	4.945543000	-3.504329000	1.054854000
C	5.502015000	-4.751965000	0.773406000
H	6.322153000	-5.103111000	1.395745000
C	5.046473000	-5.565995000	-0.271520000
C	3.985878000	-5.087108000	-1.040704000
H	3.598741000	-5.693950000	-1.857594000
C	-5.960465000	-3.757265000	-1.588619000

H	-5.473026000	-4.413651000	-0.874075000
H	-6.339524000	-2.893103000	-1.053802000
H	-6.806166000	-4.287741000	-2.016080000
C	4.045466000	4.408418000	0.176870000
H	3.424906000	5.144469000	0.710536000
H	4.943749000	4.283012000	0.801493000
Si	4.581897000	5.249180000	-1.452634000
C	5.959701000	4.307368000	-2.360693000
H	6.811418000	4.109583000	-1.698849000
H	5.596917000	3.347956000	-2.743865000
H	6.328470000	4.894432000	-3.210860000
C	5.242197000	6.976336000	-0.998086000
H	6.105493000	6.907193000	-0.325187000
H	5.561812000	7.524994000	-1.892119000
H	4.475045000	7.576668000	-0.494675000
C	3.097731000	5.446995000	-2.620486000
H	2.676288000	4.472664000	-2.892536000
H	2.302396000	6.043212000	-2.157989000
H	3.396562000	5.951977000	-3.546831000
N	2.313963000	0.729544000	-1.474635000
C	3.670979000	1.057801000	-1.406812000
C	1.828394000	0.291343000	-2.667429000
C	4.541638000	0.488921000	-2.402058000
C	4.132369000	1.954373000	-0.442088000
C	2.611716000	-0.061017000	-3.742524000
H	0.743734000	0.205901000	-2.710538000
C	4.021461000	-0.032805000	-3.555027000
H	5.616217000	0.571720000	-2.260523000
C	3.286619000	3.067767000	0.109028000
H	2.164536000	-0.390041000	-4.674607000
H	4.683841000	-0.396467000	-4.337310000
H	2.932440000	2.843935000	1.130374000
H	2.382337000	3.167744000	-0.503941000
C	-2.219022000	1.731310000	-0.298245000
C	-1.611421000	2.574650000	0.617043000
C	-1.895600000	1.895344000	-1.653394000
C	-0.723145000	3.575493000	0.211204000
H	-1.823627000	2.482028000	1.669712000
C	-1.019584000	2.875591000	-2.079965000
H	-2.354309000	1.245968000	-2.385693000
C	-0.440240000	3.723024000	-1.133079000
H	0.234578000	4.502673000	-1.459056000
C	-3.328119000	0.383417000	1.625989000
C	-3.804209000	1.381951000	2.489176000

C	-3.007089000	-0.843674000	2.177787000
C	-3.934225000	1.169372000	3.847768000
H	-4.102385000	2.336160000	2.078500000
C	-3.130737000	-1.087258000	3.549681000
H	-2.687096000	-1.649339000	1.536446000
C	-3.588268000	-0.078024000	4.373568000
H	-3.696675000	-0.256912000	5.435099000
C	-4.721069000	1.182235000	-0.284453000
C	-4.944771000	2.258904000	-1.123660000
C	-5.844374000	0.549529000	0.270940000
C	-6.237567000	2.703036000	-1.421212000
H	-4.114348000	2.788287000	-1.563066000
C	-7.131056000	0.965789000	-0.007930000
H	-5.702568000	-0.287135000	0.939721000
C	-7.319832000	2.053059000	-0.864143000
H	-8.324207000	2.388599000	-1.086077000
C	-0.694717000	3.051602000	-3.562078000
H	0.366387000	2.898314000	-3.743253000
H	-1.250128000	2.342383000	-4.166974000
H	-0.945663000	4.056210000	-3.894611000
C	-0.114561000	4.512183000	1.253732000
H	0.353373000	3.948277000	2.056072000
H	0.635446000	5.154588000	0.804968000
H	-0.882589000	5.143243000	1.696755000
C	-4.460558000	2.267383000	4.770096000
H	-3.718129000	2.531415000	5.519937000
H	-4.707801000	3.160656000	4.206051000
H	-5.353845000	1.934838000	5.293551000
C	-2.759630000	-2.455547000	4.118419000
H	-1.679257000	-2.557233000	4.200966000
H	-3.185347000	-2.592455000	5.107321000
H	-3.120309000	-3.253061000	3.474735000
C	-6.427243000	3.898229000	-2.353506000
H	-7.479526000	4.137326000	-2.467192000
H	-5.916615000	4.775758000	-1.963897000
H	-6.016226000	3.687645000	-3.338222000
C	-8.337907000	0.257616000	0.604545000
H	-8.966467000	-0.173780000	-0.171348000
H	-8.022972000	-0.539336000	1.270152000
H	-8.947805000	0.956465000	1.172155000
C	2.595517000	1.258667000	3.127939000
C	2.235465000	1.909112000	4.337016000
C	0.954424000	1.839287000	4.834293000
C	-0.010353000	1.120677000	4.113722000

C	0.387259000	0.514203000	2.938533000
N	1.642165000	0.554430000	2.433357000
H	0.697789000	2.336136000	5.766432000
H	3.005483000	2.459973000	4.868885000
H	-1.039200000	1.038317000	4.444731000
H	-0.344967000	-0.032826000	2.349965000
C	3.957767000	1.388829000	2.686160000
H	4.519081000	2.147896000	3.228609000
C	4.585176000	0.732609000	1.668132000
H	5.642992000	0.915649000	1.507078000
H	4.199282000	-0.167678000	1.208489000
H	5.203452000	2.141710000	-0.477689000
C	-4.524896000	-4.611553000	-3.468590000
H	-3.856483000	-4.368829000	-4.288068000
H	-4.021825000	-5.308643000	-2.806392000
H	-5.395729000	-5.110310000	-3.882580000
C	5.492079000	-2.645367000	2.199739000
H	6.103241000	-1.830585000	1.818169000
H	4.685186000	-2.205328000	2.779647000
H	6.107209000	-3.243509000	2.864848000
C	5.705946000	-6.921389000	-0.561680000
H	6.684236000	-6.787303000	-1.019680000
H	5.845484000	-7.490638000	0.353844000
H	5.095460000	-7.508856000	-1.240329000

P2^F_{iso}, $E_{(\text{SCF Done})} = -3280.94012003 \text{ a.u.}$

Y	-1.355216000	0.971966000	0.189578000
N	-0.492146000	3.302460000	-0.862652000
C	-0.035312000	4.194613000	0.217686000
H	-0.891824000	4.794918000	0.538567000
H	0.739648000	4.893734000	-0.138497000
C	0.509397000	3.418635000	1.406026000
H	1.385591000	2.838876000	1.121981000
H	0.793626000	4.106730000	2.212671000
O	-0.446513000	2.474948000	1.906256000
C	-1.338480000	2.996953000	2.895323000
H	-1.951363000	2.161030000	3.234650000
H	-1.981053000	3.779755000	2.478745000
H	-0.757876000	3.391485000	3.737358000
O	0.705366000	0.581350000	-0.372357000
C	1.858229000	1.116711000	-0.746209000
C	1.860015000	2.381412000	-1.387643000
C	0.577034000	3.022312000	-1.849252000
H	0.836858000	3.967311000	-2.358419000

H	0.110582000	2.391245000	-2.618838000
C	3.118732000	0.474917000	-0.529772000
C	4.275703000	1.150030000	-0.925862000
H	5.222599000	0.653666000	-0.774046000
C	4.295158000	2.421268000	-1.515212000
C	3.055316000	3.012307000	-1.739826000
H	2.984242000	3.982260000	-2.221681000
C	3.194026000	-0.965774000	0.123269000
C	5.660756000	3.081708000	-1.900549000
C	6.398731000	2.188437000	-2.936898000
H	7.345220000	2.640989000	-3.217541000
H	5.798380000	2.070082000	-3.833817000
H	6.602233000	1.203351000	-2.530936000
O	-3.017103000	2.320816000	0.177671000
C	-3.437807000	3.566241000	0.041181000
C	-2.758039000	4.446282000	-0.824519000
C	-1.610524000	3.921727000	-1.635581000
H	-1.966050000	3.144849000	-2.328896000
H	-1.209876000	4.740295000	-2.258378000
C	-4.562697000	4.043264000	0.762259000
C	-4.956235000	5.369988000	0.598462000
H	-5.818819000	5.726529000	1.157164000
C	-4.286477000	6.258717000	-0.255825000
C	-3.184788000	5.770951000	-0.958126000
H	-2.642289000	6.431565000	-1.632524000
C	6.544269000	3.232480000	-0.630344000
H	6.047404000	3.854044000	0.108403000
H	6.751263000	2.267725000	-0.179945000
H	7.492277000	3.697379000	-0.884288000
C	-4.374016000	-3.819373000	0.378807000
H	-3.749601000	-4.496631000	0.980930000
H	-5.008829000	-3.299171000	1.107254000
Si	-5.456331000	-4.977536000	-0.685639000
C	-6.919260000	-4.097152000	-1.530503000
H	-7.492595000	-3.498627000	-0.812925000
H	-6.593947000	-3.431934000	-2.338587000
H	-7.602022000	-4.835039000	-1.969175000
C	-6.166958000	-6.301564000	0.478510000
H	-6.791112000	-5.847284000	1.257062000
H	-6.786993000	-7.020803000	-0.069556000
H	-5.366653000	-6.860432000	0.977583000
C	-4.401312000	-5.826131000	-2.021313000
H	-3.976646000	-5.100466000	-2.725178000
H	-3.569395000	-6.381751000	-1.572862000

H	-5.003639000	-6.536976000	-2.599385000
N	-2.230691000	-0.371754000	-1.804649000
C	-3.407714000	-1.005520000	-2.031319000
C	-1.464722000	-0.042199000	-2.862916000
C	-3.854526000	-1.213678000	-3.343619000
C	-4.191008000	-1.563016000	-0.870874000
C	-1.840950000	-0.235046000	-4.183857000
H	-0.491985000	0.378947000	-2.622589000
C	-3.082719000	-0.817427000	-4.427097000
H	-4.811866000	-1.701586000	-3.498731000
C	-3.452271000	-2.800709000	-0.309662000
H	-1.177410000	0.062138000	-4.989311000
H	-3.434237000	-0.977921000	-5.442939000
H	-2.693235000	-2.450556000	0.397767000
H	-2.911235000	-3.294205000	-1.128194000
C	2.098573000	-1.860084000	-0.545071000
C	1.299736000	-2.749594000	0.158118000
C	1.962028000	-1.825510000	-1.939397000
C	0.414975000	-3.612035000	-0.493535000
H	1.358524000	-2.803613000	1.233090000
C	1.086420000	-2.663183000	-2.607644000
H	2.570860000	-1.139242000	-2.511219000
C	0.316769000	-3.564312000	-1.872696000
H	-0.356485000	-4.236168000	-2.388217000
C	3.033254000	-0.888734000	1.676420000
C	3.261668000	-2.035990000	2.448337000
C	2.771708000	0.295529000	2.343880000
C	3.199900000	-2.009642000	3.829030000
H	3.517878000	-2.962855000	1.955357000
C	2.709747000	0.351973000	3.739047000
H	2.648836000	1.208091000	1.782952000
C	2.917232000	-0.802602000	4.469548000
H	2.877098000	-0.769438000	5.550259000
C	4.609626000	-1.607762000	-0.120000000
C	4.851911000	-2.593706000	-1.059446000
C	5.693322000	-1.178727000	0.662571000
C	6.126033000	-3.143773000	-1.236349000
H	4.049948000	-2.968100000	-1.675404000
C	6.961256000	-1.702590000	0.506787000
H	5.533626000	-0.417285000	1.412368000
C	7.170425000	-2.693646000	-0.455173000
H	8.159781000	-3.112682000	-0.582388000
C	1.004048000	-2.646173000	-4.133277000
H	-0.014291000	-2.815492000	-4.470551000

H	1. 347457000	-1. 696426000	-4. 531201000
H	1. 627330000	-3. 430870000	-4. 558528000
C	-0. 376686000	-4. 631786000	0. 323327000
H	-0. 833714000	-4. 163767000	1. 190522000
H	-1. 156639000	-5. 089698000	-0. 275410000
H	0. 281811000	-5. 421216000	0. 680978000
C	3. 434809000	-3. 276236000	4. 649492000
H	2. 497291000	-3. 644141000	5. 061962000
H	3. 864839000	-4. 060996000	4. 035632000
H	4. 107543000	-3. 079968000	5. 480083000
C	2. 408208000	1. 673545000	4. 442585000
H	1. 333611000	1. 826573000	4. 521161000
H	2. 819871000	1. 680127000	5. 447096000
H	2. 827647000	2. 510820000	3. 892563000
C	6. 337094000	-4. 232285000	-2. 287228000
H	7. 368197000	-4. 570196000	-2. 292868000
H	5. 697256000	-5. 088950000	-2. 088748000
H	6. 093598000	-3. 861836000	-3. 280417000
C	8. 125544000	-1. 215939000	1. 367407000
H	8. 905455000	-0. 777430000	0. 748844000
H	7. 794276000	-0. 467691000	2. 079942000
H	8. 567925000	-2. 041758000	1. 919588000
C	-3. 273374000	-0. 805684000	2. 417546000
C	-3. 344936000	-1. 209586000	3. 814006000
C	-2. 232135000	-1. 375950000	4. 572941000
C	-0. 943609000	-1. 129464000	4. 002748000
C	-0. 910860000	-0. 662410000	2. 719132000
N	-2. 001682000	-0. 434156000	1. 925458000
H	-2. 319014000	-1. 698174000	5. 608724000
H	-4. 332730000	-1. 403743000	4. 224893000
H	-0. 027007000	-1. 280645000	4. 561146000
H	0. 050291000	-0. 425889000	2. 262167000
C	-4. 410447000	-0. 816078000	1. 650924000
H	-5. 320680000	-1. 118448000	2. 164215000
C	-4. 539173000	-0. 464117000	0. 204415000
H	-5. 574748000	-0. 156019000	0. 012386000
H	-3. 969052000	0. 441930000	-0. 024948000
H	-5. 134895000	-1. 923687000	-1. 295449000
C	5. 466764000	4. 488472000	-2. 524133000
H	4. 884274000	4. 436523000	-3. 438077000
H	4. 966909000	5. 159032000	-1. 832762000
H	6. 434289000	4. 916683000	-2. 767075000
C	-5. 319794000	3. 087270000	1. 688245000
H	-5. 816283000	2. 306739000	1. 116843000

H	-4.641799000	2.596060000	2.382303000
H	-6.071263000	3.622880000	2.259887000
C	-4.765288000	7.709038000	-0.410753000
H	-5.756539000	7.745663000	-0.858005000
H	-4.821170000	8.206529000	0.554779000
H	-4.087616000	8.271787000	-1.044911000

C3^F_{syn}, $E_{(\text{SCF Done})} = -3606.471369$ a.u.

Y	-0.552701000	1.667783000	0.265044000
N	1.122613000	3.433191000	-0.702125000
C	1.992439000	4.004745000	0.341950000
H	1.515876000	4.917958000	0.710310000
H	2.974161000	4.290372000	-0.069334000
C	2.204051000	3.038938000	1.495393000
H	2.733591000	2.152259000	1.157952000
H	2.794751000	3.518344000	2.287421000
O	0.963632000	2.577560000	2.042910000
C	0.433011000	3.427680000	3.059725000
H	-0.470488000	2.947974000	3.436542000
H	0.180804000	4.417275000	2.665942000
H	1.162623000	3.521382000	3.873687000
O	1.213482000	0.420162000	-0.252838000
C	2.463760000	0.513385000	-0.671200000
C	2.880804000	1.679140000	-1.369593000
C	1.892478000	2.744045000	-1.769827000
H	2.439629000	3.508550000	-2.348394000
H	1.144492000	2.320729000	-2.452082000
C	3.445771000	-0.510245000	-0.449626000
C	4.729719000	-0.316104000	-0.966071000
H	5.445793000	-1.115194000	-0.843424000
C	5.154463000	0.836648000	-1.639373000
C	4.194812000	1.828142000	-1.818576000
H	4.440745000	2.745651000	-2.343953000
C	3.048659000	-1.873359000	0.252539000
C	6.629068000	0.942601000	-2.152739000
C	6.912168000	-0.198439000	-3.169952000
H	7.931117000	-0.130200000	-3.539554000
H	6.236977000	-0.129242000	-4.017427000
H	6.783922000	-1.173001000	-2.711285000
O	-1.461228000	3.592155000	0.644196000
C	-1.332815000	4.894530000	0.486294000
C	-0.434324000	5.426286000	-0.466473000
C	0.330509000	4.502970000	-1.373241000
H	-0.360327000	3.990808000	-2.054903000

H	1.006001000	5.107554000	-2.003656000
C	-2.105148000	5.796583000	1.267744000
C	-1.946017000	7.168708000	1.090499000
H	-2.546964000	7.844046000	1.696049000
C	-1.046523000	7.707708000	0.158718000
C	-0.301525000	6.811496000	-0.607046000
H	0.401489000	7.195923000	-1.344541000
C	7.611416000	0.816375000	-0.954344000
H	7.432947000	1.605655000	-0.230362000
H	7.496469000	-0.138251000	-0.452390000
H	8.638472000	0.895981000	-1.298277000
C	-6.160559000	-2.181144000	1.691293000
H	-6.073661000	-2.311938000	2.780786000
H	-6.817791000	-1.306962000	1.567229000
Si	-7.112286000	-3.748860000	1.142654000
C	-8.086265000	-3.543879000	-0.475253000
H	-8.739135000	-2.663889000	-0.432642000
H	-7.431164000	-3.436614000	-1.344430000
H	-8.723567000	-4.421648000	-0.639695000
C	-8.381031000	-4.105679000	2.518658000
H	-9.074910000	-3.265900000	2.646624000
H	-8.977042000	-4.995777000	2.284046000
H	-7.886498000	-4.279481000	3.481849000
C	-5.921946000	-5.219722000	0.999109000
H	-5.173515000	-5.032280000	0.221921000
H	-5.393400000	-5.395350000	1.943683000
H	-6.462779000	-6.138178000	0.741598000
N	-4.485170000	-2.948878000	-1.621360000
C	-5.051251000	-1.751783000	-1.403728000
C	-4.738276000	-3.574600000	-2.773913000
C	-5.888305000	-1.155617000	-2.360007000
C	-4.691535000	-1.014704000	-0.132617000
C	-5.555056000	-3.058526000	-3.776903000
H	-4.259849000	-4.545643000	-2.900851000
C	-6.142372000	-1.813727000	-3.557880000
H	-6.333890000	-0.185698000	-2.154465000
C	-4.753650000	-1.866407000	1.142078000
H	-5.725781000	-3.616298000	-4.693255000
H	-6.793571000	-1.366674000	-4.305615000
H	-4.205240000	-1.308467000	1.911046000
H	-4.187941000	-2.788908000	0.970239000
C	1.882655000	-2.481840000	-0.588932000
C	0.663028000	-2.891225000	-0.061283000
C	2.100413000	-2.679202000	-1.953937000

C	-0.287002000	-3.541379000	-0.845374000
H	0.439291000	-2.727034000	0.980431000
C	1.167467000	-3.316625000	-2.758899000
H	3.034704000	-2.354455000	-2.390386000
C	-0.022695000	-3.755267000	-2.191308000
H	-0.750175000	-4.271892000	-2.803183000
C	2.713737000	-1.694709000	1.768661000
C	2.309669000	-2.803530000	2.519381000
C	2.997849000	-0.520593000	2.452974000
C	2.144806000	-2.734842000	3.893153000
H	2.152249000	-3.750754000	2.024531000
C	2.859744000	-0.430186000	3.837714000
H	3.386250000	0.325902000	1.910004000
C	2.419638000	-1.536577000	4.546046000
H	2.313146000	-1.477002000	5.621031000
C	4.259580000	-2.878867000	0.298892000
C	4.253234000	-4.120933000	-0.308320000
C	5.382034000	-2.541964000	1.073341000
C	5.332071000	-5.004577000	-0.185805000
H	3.402323000	-4.439456000	-0.889232000
C	6.459757000	-3.392683000	1.208170000
H	5.402783000	-1.588775000	1.581706000
C	6.427601000	-4.633186000	0.564774000
H	7.266922000	-5.308209000	0.666689000
C	1.477969000	-3.587688000	-4.230727000
H	2.058946000	-2.778362000	-4.663441000
H	2.058479000	-4.502550000	-4.335576000
H	0.565781000	-3.707500000	-4.807254000
C	-1.575715000	-4.068288000	-0.218325000
H	-1.639941000	-3.774012000	0.823590000
H	-2.454900000	-3.693663000	-0.736877000
H	-1.598428000	-5.154908000	-0.264750000
C	1.673532000	-3.954435000	4.682760000
H	1.878761000	-4.870743000	4.138336000
H	2.169115000	-4.006797000	5.647857000
H	0.600919000	-3.903585000	4.861754000
C	3.200032000	0.863531000	4.575238000
H	2.294380000	1.395447000	4.858748000
H	3.757012000	0.653659000	5.484283000
H	3.797594000	1.520297000	3.951663000
C	5.275170000	-6.362613000	-0.883131000
H	6.160533000	-6.949323000	-0.661034000
H	4.401867000	-6.925034000	-0.561417000
H	5.209069000	-6.239669000	-1.961857000

C	7. 673938000	-2. 999810000	2. 047488000
H	8. 569476000	-2. 952624000	1. 431806000
H	7. 527274000	-2. 029441000	2. 510291000
H	7. 852097000	-3. 730228000	2. 833149000
C	-2. 588667000	0. 750167000	1. 924541000
C	-3. 239525000	1. 254104000	3. 091121000
C	-2. 692675000	1. 024862000	4. 332648000
C	-1. 464866000	0. 336407000	4. 447282000
C	-0. 810703000	-0. 003702000	3. 280570000
N	-1. 317138000	0. 233271000	2. 053858000
H	-3. 218518000	1. 352084000	5. 227294000
H	-4. 200811000	1. 748205000	2. 982786000
H	-1. 025176000	0. 114939000	5. 414265000
H	0. 177510000	-0. 453499000	3. 298093000
C	-3. 081141000	0. 861993000	0. 590959000
H	-3. 934541000	1. 544316000	0. 528283000
C	-3. 281184000	-0. 350279000	-0. 305753000
H	-3. 190991000	-0. 058809000	-1. 359098000
H	-2. 511827000	-1. 113708000	-0. 129657000
H	-5. 409426000	-0. 187518000	-0. 029512000
C	6. 899759000	2. 297232000	-2. 858014000
H	6. 260711000	2. 423000000	-3. 725816000
H	6. 734755000	3. 131015000	-2. 183451000
H	7. 931751000	2. 335470000	-3. 192897000
C	-3. 107954000	5. 225352000	2. 275279000
H	-3. 793087000	4. 536684000	1. 786825000
H	-2. 602340000	4. 673331000	3. 064719000
H	-3. 686974000	6. 020655000	2. 734442000
C	-0. 897804000	9. 227241000	-0. 002322000
H	-0. 553210000	9. 686804000	0. 921775000
H	-0. 182410000	9. 462368000	-0. 784005000
H	-1. 848663000	9. 686763000	-0. 263109000
C	-1. 990803000	1. 976731000	-3. 302437000
C	-2. 028610000	1. 518875000	-4. 629247000
C	-1. 357159000	0. 362627000	-4. 995149000
C	-0. 641524000	-0. 317433000	-4. 017060000
C	-0. 614086000	0. 210080000	-2. 731019000
N	-1. 254344000	1. 334412000	-2. 358554000
H	-1. 394340000	0. 000537000	-6. 019075000
H	-2. 610454000	2. 075750000	-5. 357795000
H	-0. 096090000	-1. 228239000	-4. 232250000
H	-0. 017298000	-0. 273302000	-1. 961389000
C	-2. 792919000	3. 169599000	-2. 998032000
H	-3. 039419000	3. 769468000	-3. 873915000

C	-3.289965000	3.524256000	-1.809086000
H	-3.102672000	2.956773000	-0.904094000
H	-3.897121000	4.420239000	-1.715196000

TS3^F_{syn}, $E_{(\text{SCF Done})} = -3606.440594$ a.u. IF = $i143.82$ cm⁻¹

Y	-0.051071000	1.783916000	0.174122000
N	1.855264000	3.272429000	-0.825803000
C	2.773320000	3.778277000	0.210988000
H	2.386694000	4.738948000	0.562542000
H	3.777654000	3.963527000	-0.203813000
C	2.892250000	2.817225000	1.381815000
H	3.321694000	1.871412000	1.061663000
H	3.539877000	3.247848000	2.157020000
O	1.614346000	2.507805000	1.950433000
C	1.207118000	3.431220000	2.962021000
H	0.265607000	3.061939000	3.368916000
H	1.060974000	4.436181000	2.554303000
H	1.961906000	3.454668000	3.757707000
O	1.492216000	0.343339000	-0.283298000
C	2.746620000	0.208894000	-0.692483000
C	3.359011000	1.269552000	-1.406191000
C	2.566034000	2.472811000	-1.854948000
H	3.249250000	3.144031000	-2.403870000
H	1.800574000	2.166142000	-2.580252000
C	3.515684000	-0.969946000	-0.440241000
C	4.834668000	-1.000565000	-0.898257000
H	5.402981000	-1.903967000	-0.732779000
C	5.468049000	0.054486000	-1.570124000
C	4.692892000	1.185081000	-1.812378000
H	5.105706000	2.033272000	-2.348874000
C	2.846740000	-2.224563000	0.256273000
C	6.959855000	-0.093628000	-2.020334000
C	7.090640000	-1.286580000	-3.008432000
H	8.121059000	-1.394077000	-3.334095000
H	6.471206000	-1.124589000	-3.885330000
H	6.784659000	-2.217076000	-2.542447000
O	-0.632371000	3.812846000	0.552649000
C	-0.355577000	5.088841000	0.332697000
C	0.562690000	5.452950000	-0.674627000
C	1.176237000	4.392342000	-1.546202000
H	0.406681000	3.926569000	-2.178207000
H	1.897253000	4.871026000	-2.230164000
C	-0.966461000	6.109360000	1.105658000
C	-0.640235000	7.440481000	0.852627000

H	-1.116312000	8.213455000	1.451825000
C	0.274389000	7.817269000	-0.140660000
C	0.865898000	6.800638000	-0.890148000
H	1.580295000	7.057487000	-1.670482000
C	7.856377000	-0.354830000	-0.777443000
H	7.780615000	0.467717000	-0.072704000
H	7.565064000	-1.267331000	-0.268573000
H	8.895707000	-0.451826000	-1.076936000
C	-6.872299000	-1.625076000	1.666137000
H	-6.858019000	-1.781038000	2.755883000
H	-7.477621000	-0.716600000	1.523326000
Si	-7.868526000	-3.130109000	1.029955000
C	-8.675526000	-2.874219000	-0.670745000
H	-9.261875000	-1.947842000	-0.693203000
H	-7.940114000	-2.828254000	-1.479076000
H	-9.360201000	-3.704242000	-0.885345000
C	-9.276335000	-3.394545000	2.286361000
H	-9.921724000	-2.510268000	2.354788000
H	-9.907284000	-4.244108000	1.998774000
H	-8.881391000	-3.596888000	3.289136000
C	-6.765458000	-4.673237000	1.000070000
H	-5.936093000	-4.537096000	0.297835000
H	-6.341165000	-4.875226000	1.990852000
H	-7.335188000	-5.558280000	0.692707000
N	-4.980974000	-2.512503000	-1.482300000
C	-5.489744000	-1.278447000	-1.355536000
C	-5.140714000	-3.152154000	-2.644288000
C	-6.173331000	-0.657721000	-2.412429000
C	-5.243161000	-0.529385000	-0.062485000
C	-5.803313000	-2.613708000	-3.744125000
H	-4.714352000	-4.153720000	-2.696310000
C	-6.331434000	-1.330123000	-3.618455000
H	-6.576734000	0.342614000	-2.278046000
C	-5.421523000	-1.367960000	1.211652000
H	-5.903449000	-3.183861000	-4.663228000
H	-6.863517000	-0.864341000	-4.444837000
H	-4.903686000	-0.822300000	2.011261000
H	-4.880467000	-2.312185000	1.085490000
C	1.508530000	-2.507477000	-0.500940000
C	0.299026000	-2.756590000	0.133241000
C	1.536560000	-2.573046000	-1.898115000
C	-0.844300000	-3.109406000	-0.584028000
H	0.223725000	-2.697185000	1.206563000
C	0.413141000	-2.911817000	-2.634715000

H	2.464173000	-2.375483000	-2.416863000
C	-0.776771000	-3.186833000	-1.965917000
H	-1.655715000	-3.467682000	-2.530624000
C	2.638489000	-2.005408000	1.789665000
C	2.141083000	-3.058454000	2.565746000
C	3.048769000	-0.855840000	2.447812000
C	2.008792000	-2.954185000	3.939714000
H	1.872891000	-3.988652000	2.085696000
C	2.942187000	-0.730875000	3.833928000
H	3.503663000	-0.056045000	1.886323000
C	2.408841000	-1.776741000	4.567130000
H	2.324133000	-1.689250000	5.642232000
C	3.787222000	-3.481780000	0.171476000
C	3.527390000	-4.585885000	-0.619011000
C	4.937514000	-3.514812000	0.976076000
C	4.381972000	-5.694174000	-0.635707000
H	2.645124000	-4.616836000	-1.238490000
C	5.798408000	-4.593509000	0.976283000
H	5.155553000	-2.672614000	1.617230000
C	5.510744000	-5.688589000	0.157127000
H	6.177927000	-6.540315000	0.152824000
C	0.489566000	-3.041377000	-4.155219000
H	1.320657000	-2.468341000	-4.554358000
H	0.633835000	-4.081347000	-4.442851000
H	-0.427720000	-2.694926000	-4.622244000
C	-2.123977000	-3.478049000	0.162688000
H	-2.164390000	-2.974973000	1.123197000
H	-3.008420000	-3.211890000	-0.408269000
H	-2.151219000	-4.550761000	0.346712000
C	1.433593000	-4.107556000	4.759169000
H	1.485789000	-5.039505000	4.205399000
H	1.976615000	-4.228449000	5.692266000
H	0.389836000	-3.919091000	5.003980000
C	3.416793000	0.535542000	4.544042000
H	2.570075000	1.149338000	4.843521000
H	3.977196000	0.286937000	5.441194000
H	4.053885000	1.128514000	3.896252000
C	4.048302000	-6.888651000	-1.527657000
H	4.787100000	-7.675174000	-1.413821000
H	3.072175000	-7.296644000	-1.276009000
H	4.022361000	-6.593105000	-2.574061000
C	7.047472000	-4.605075000	1.855324000
H	7.946234000	-4.682518000	1.247536000
H	7.113080000	-3.697979000	2.447101000

H	7.033600000	-5.455293000	2.533207000
C	-2.770676000	1.248673000	1.951816000
C	-3.114446000	1.778942000	3.242145000
C	-2.331776000	1.523144000	4.335981000
C	-1.141190000	0.766874000	4.185439000
C	-0.764007000	0.437187000	2.903815000
N	-1.486503000	0.730704000	1.789903000
H	-2.637738000	1.873285000	5.319385000
H	-4.058531000	2.307503000	3.346079000
H	-0.522795000	0.493208000	5.033454000
H	0.187757000	-0.058861000	2.719524000
C	-3.714237000	1.230862000	0.909976000
H	-4.665064000	1.679041000	1.198028000
C	-3.835074000	0.140096000	-0.114221000
H	-3.700836000	0.530297000	-1.135977000
H	-3.058956000	-0.620816000	0.032255000
H	-5.972528000	0.295079000	-0.034032000
C	7.478961000	1.183409000	-2.731062000
H	6.907725000	1.393194000	-3.629373000
H	7.424332000	2.047118000	-2.076447000
H	8.516646000	1.044866000	-3.018268000
C	-1.989192000	5.728072000	2.181234000
H	-2.911370000	5.368321000	1.730310000
H	-1.609520000	4.934341000	2.819246000
H	-2.228438000	6.585548000	2.802399000
C	0.597741000	9.296970000	-0.390473000
H	0.928142000	9.783626000	0.524306000
H	1.382854000	9.398569000	-1.132982000
H	-0.279409000	9.831211000	-0.749828000
C	-2.363135000	2.058096000	-2.592922000
C	-2.591607000	1.870477000	-3.983908000
C	-1.708230000	1.172218000	-4.771448000
C	-0.575152000	0.605672000	-4.167776000
C	-0.392778000	0.818448000	-2.816535000
N	-1.214650000	1.554216000	-2.024586000
H	-1.895248000	1.048421000	-5.835114000
H	-3.493712000	2.297496000	-4.411848000
H	0.140004000	0.011794000	-4.725360000
H	0.457131000	0.367234000	-2.311330000
C	-3.395169000	2.722929000	-1.847092000
H	-4.328451000	2.817620000	-2.400281000
C	-3.377525000	3.147185000	-0.546629000
H	-2.463990000	3.349859000	-0.007541000
H	-4.262083000	3.644124000	-0.157947000

P3^F_{syn}, $E_{\text{(SCF Done)}} = 3606.497749 \text{ a.u.}$

Y	-0.142160000	1.788138000	0.287491000
N	1.393451000	3.339853000	-1.038855000
C	2.384147000	4.036394000	-0.197694000
H	1.937391000	4.979403000	0.130777000
H	3.288029000	4.287700000	-0.775930000
C	2.791852000	3.214107000	1.015276000
H	3.275342000	2.289320000	0.709299000
H	3.495421000	3.784841000	1.636670000
O	1.661141000	2.830219000	1.810348000
C	1.284300000	3.815121000	2.771248000
H	0.431637000	3.415043000	3.321910000
H	0.986371000	4.754425000	2.295286000
H	2.116849000	3.991876000	3.464225000
O	1.472480000	0.440336000	-0.231360000
C	2.656206000	0.401710000	-0.823299000
C	3.031312000	1.464791000	-1.684041000
C	2.031793000	2.515125000	-2.099346000
H	2.529190000	3.195498000	-2.811386000
H	1.205937000	2.046055000	-2.651949000
C	3.583645000	-0.669166000	-0.631569000
C	4.831197000	-0.574506000	-1.253475000
H	5.524600000	-1.391236000	-1.116359000
C	5.239546000	0.498512000	-2.057602000
C	4.300565000	1.506107000	-2.264139000
H	4.528481000	2.350179000	-2.907082000
C	3.174095000	-1.947034000	0.210591000
C	6.672133000	0.498065000	-2.688279000
C	6.831799000	-0.734449000	-3.622038000
H	7.820227000	-0.740297000	-4.071938000
H	6.094692000	-0.706420000	-4.418738000
H	6.704690000	-1.661307000	-3.073040000
O	-0.941819000	3.748923000	0.648483000
C	-0.854278000	5.015595000	0.282848000
C	-0.120295000	5.376955000	-0.868396000
C	0.485695000	4.307717000	-1.734531000
H	-0.304060000	3.702524000	-2.202271000
H	1.041736000	4.790104000	-2.555584000
C	-1.482621000	6.036964000	1.041101000
C	-1.348373000	7.364773000	0.641720000
H	-1.837841000	8.136438000	1.232017000
C	-0.612450000	7.739054000	-0.491718000
C	-0.006204000	6.722772000	-1.230081000

H	0.567197000	6.978095000	-2.119688000
C	7.738937000	0.429278000	-1.559462000
H	7.646501000	1.282656000	-0.894465000
H	7.629127000	-0.474899000	-0.970482000
H	8.738126000	0.436113000	-1.984796000
C	-7.578972000	-1.219174000	0.945728000
H	-8.106788000	-1.122631000	1.907062000
H	-7.716190000	-0.244969000	0.452596000
Si	-8.625169000	-2.525515000	0.014822000
C	-8.428053000	-2.494496000	-1.872356000
H	-8.578389000	-1.483169000	-2.268196000
H	-7.441376000	-2.839399000	-2.193636000
H	-9.180437000	-3.146342000	-2.333479000
C	-10.440760000	-2.097424000	0.401957000
H	-10.692201000	-1.085550000	0.061543000
H	-11.124706000	-2.794350000	-0.096925000
H	-10.641529000	-2.146561000	1.478873000
C	-8.238902000	-4.258878000	0.683639000
H	-7.190000000	-4.512697000	0.497718000
H	-8.417564000	-4.317216000	1.764068000
H	-8.867007000	-5.015961000	0.199277000
N	-4.940950000	-3.280328000	-0.673536000
C	-4.973175000	-1.976399000	-0.985659000
C	-4.765414000	-4.165146000	-1.659740000
C	-4.813599000	-1.528054000	-2.304055000
C	-5.101499000	-0.985138000	0.158136000
C	-4.606013000	-3.813957000	-2.997352000
H	-4.751276000	-5.213133000	-1.360654000
C	-4.627399000	-2.458132000	-3.320275000
H	-4.814400000	-0.463594000	-2.519235000
C	-6.083905000	-1.447455000	1.247602000
H	-4.467345000	-4.578279000	-3.756707000
H	-4.499623000	-2.127876000	-4.348120000
H	-5.846996000	-0.899608000	2.170112000
H	-5.883886000	-2.503301000	1.463522000
C	1.742110000	-2.383390000	-0.245893000
C	0.757379000	-2.825220000	0.624576000
C	1.455761000	-2.407292000	-1.617720000
C	-0.466498000	-3.311998000	0.159065000
H	0.926092000	-2.817601000	1.688815000
C	0.245529000	-2.869698000	-2.103178000
H	2.206151000	-2.068897000	-2.318126000
C	-0.713689000	-3.330330000	-1.201104000
H	-1.656681000	-3.709109000	-1.571876000

C	3.248495000	-1.671539000	1.747902000
C	3.102986000	-2.739343000	2.644725000
C	3.557218000	-0.428302000	2.273784000
C	3.224360000	-2.567382000	4.010951000
H	2.916627000	-3.731388000	2.258966000
C	3.696124000	-0.228268000	3.650187000
H	3.736429000	0.400849000	1.608615000
C	3.517515000	-1.297058000	4.507999000
H	3.629918000	-1.154909000	5.574702000
C	4.185750000	-3.122257000	-0.050005000
C	3.899920000	-4.211556000	-0.852880000
C	5.444377000	-3.085182000	0.570231000
C	4.826492000	-5.240900000	-1.051224000
H	2.941538000	-4.291099000	-1.341166000
C	6.377889000	-4.086274000	0.389607000
H	5.693258000	-2.250310000	1.209535000
C	6.057142000	-5.170258000	-0.431111000
H	6.781081000	-5.961107000	-0.576294000
C	-0.035399000	-2.912086000	-3.603959000
H	0.759604000	-2.426960000	-4.160649000
H	-0.115228000	-3.940424000	-3.950410000
H	-0.971690000	-2.410471000	-3.833875000
C	-1.482081000	-3.880329000	1.149084000
H	-1.511945000	-3.289313000	2.059528000
H	-2.477595000	-3.905545000	0.717594000
H	-1.210127000	-4.897626000	1.425693000
C	3.052655000	-3.744255000	4.969507000
H	2.976770000	-4.679215000	4.424151000
H	3.895466000	-3.812007000	5.652654000
H	2.151391000	-3.626255000	5.567680000
C	4.041626000	1.155157000	4.198395000
H	3.138136000	1.728214000	4.397245000
H	4.594962000	1.074952000	5.129139000
H	4.642609000	1.714308000	3.487864000
C	4.459521000	-6.422300000	-1.947469000
H	5.266771000	-7.146497000	-1.983237000
H	3.566622000	-6.922379000	-1.579714000
H	4.255687000	-6.087285000	-2.961950000
C	7.743546000	-4.022151000	1.070762000
H	8.541684000	-3.992930000	0.332323000
H	7.824167000	-3.138194000	1.694829000
H	7.904248000	-4.897724000	1.695361000
C	-2.385674000	0.221598000	2.616118000
C	-2.635974000	-0.373630000	3.860424000

C	-1.592560000	-0.691683000	4.718014000
C	-0.288410000	-0.408279000	4.318601000
C	-0.106361000	0.195350000	3.084174000
N	-1.115800000	0.519617000	2.251113000
H	-1.792637000	-1.157421000	5.679351000
H	-3.662585000	-0.594928000	4.136195000
H	0.570300000	-0.645243000	4.938058000
H	0.897333000	0.429755000	2.737474000
C	-3.541602000	0.463438000	1.669998000
H	-4.430143000	0.452364000	2.311711000
C	-3.673875000	-0.748066000	0.715611000
H	-2.973609000	-0.613900000	-0.115261000
H	-3.374982000	-1.662173000	1.243034000
H	-5.446529000	-0.032599000	-0.262382000
C	6.935921000	1.777260000	-3.524659000
H	6.240180000	1.855337000	-4.353548000
H	6.848990000	2.670390000	-2.914494000
H	7.941412000	1.745713000	-3.932690000
C	-2.316632000	5.644273000	2.264663000
H	-3.157065000	5.019231000	1.971721000
H	-1.723865000	5.078434000	2.979954000
H	-2.703988000	6.526500000	2.764732000
C	-0.499163000	9.213617000	-0.903491000
H	-0.136826000	9.822803000	-0.078610000
H	0.185831000	9.327982000	-1.737646000
H	-1.467193000	9.609024000	-1.204640000
C	-2.957892000	1.710507000	-1.541268000
C	-3.410257000	1.930554000	-2.908499000
C	-2.709915000	1.463135000	-3.974908000
C	-1.488618000	0.749206000	-3.761683000
C	-1.029111000	0.666495000	-2.475640000
N	-1.652404000	1.195905000	-1.377532000
H	-3.076358000	1.629804000	-4.986073000
H	-4.346044000	2.467213000	-3.046785000
H	-0.928157000	0.312167000	-4.580655000
H	-0.086154000	0.165275000	-2.263410000
C	-3.789224000	1.987268000	-0.488552000
H	-4.758553000	2.405997000	-0.749803000
C	-3.490031000	1.870777000	0.975813000
H	-2.532805000	2.348554000	1.215892000
H	-4.208255000	2.506404000	1.508297000

C3^F_{iso}, $E_{(\text{SCF Done})} = -3606.482851$ a.u.

Y	-0.644245000	1.728270000	0.104726000
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N	1. 157282000	3. 402267000	-0. 898415000
C	2. 082750000	3. 912681000	0. 131787000
H	1. 711709000	4. 886894000	0. 464291000
H	3. 090074000	4. 072489000	-0. 283220000
C	2. 179675000	2. 972420000	1. 323112000
H	2. 589560000	2. 005536000	1. 036632000
H	2. 828334000	3. 406072000	2. 096694000
O	0. 887571000	2. 708314000	1. 879992000
C	0. 463409000	3. 723215000	2. 788613000
H	-0. 545944000	3. 470999000	3. 108457000
H	0. 444143000	4. 708994000	2. 313090000
H	1. 136220000	3. 739020000	3. 656336000
O	1. 029425000	0. 412040000	-0. 462225000
C	2. 297748000	0. 432372000	-0. 837906000
C	2. 797761000	1. 556058000	-1. 548201000
C	1. 884550000	2. 676690000	-1. 970858000
H	2. 487212000	3. 407892000	-2. 537804000
H	1. 120524000	2. 309687000	-2. 664711000
C	3. 216501000	-0. 625172000	-0. 537354000
C	4. 550907000	-0. 468964000	-0. 924417000
H	5. 245914000	-1. 251120000	-0. 655756000
C	5. 055833000	0. 635555000	-1. 622417000
C	4. 140462000	1. 640448000	-1. 921454000
H	4. 452348000	2. 528984000	-2. 461225000
C	2. 771542000	-1. 867374000	0. 335933000
C	6. 571302000	0. 688278000	-2. 009656000
C	6. 925631000	1. 985505000	-2. 782493000
H	7. 981116000	1. 982989000	-3. 036525000
H	6. 727432000	2. 867355000	-2. 182143000
H	6. 358568000	2. 060373000	-3. 704563000
C	6. 921249000	-0. 525877000	-2. 915228000
H	7. 969527000	-0. 495994000	-3. 197535000
H	6. 323718000	-0. 509588000	-3. 821640000
H	6. 735975000	-1. 463427000	-2. 402200000
O	-1. 527811000	3. 674565000	0. 350473000
C	-1. 304377000	4. 969333000	0. 234209000
C	-0. 317745000	5. 460696000	-0. 651093000
C	0. 421046000	4. 517104000	-1. 559452000
H	-0. 280446000	4. 041307000	-2. 255368000
H	1. 128851000	5. 101190000	-2. 173897000
C	-2. 053033000	5. 902215000	1. 001458000
C	-1. 784664000	7. 263362000	0. 880327000
H	-2. 368414000	7. 962600000	1. 475547000
C	-0. 795731000	7. 762475000	0. 019768000

C	-0.076441000	6.836556000	-0.734695000
H	0.690990000	7.189791000	-1.421982000
N	-1.425195000	1.648475000	-2.572566000
C	-2.222274000	2.403038000	-3.371305000
C	-0.673518000	0.703086000	-3.164983000
C	-2.205564000	2.252260000	-4.768327000
C	-3.141722000	3.404922000	-2.818640000
C	-0.629812000	0.479710000	-4.537453000
H	-0.043754000	0.123405000	-2.496127000
C	-1.407510000	1.286651000	-5.361607000
H	-2.840856000	2.894374000	-5.371530000
H	-3.417493000	4.197786000	-3.513019000
C	-3.700559000	3.371362000	-1.605805000
H	0.019128000	-0.289673000	-4.940512000
H	-1.394461000	1.164526000	-6.441486000
H	-3.486483000	2.580834000	-0.897517000
H	-4.391071000	4.149073000	-1.293499000
C	3.969262000	-2.864498000	0.540984000
C	4.452729000	-3.564182000	-0.576564000
C	4.539737000	-3.141639000	1.768684000
C	5.474277000	-4.485372000	-0.473688000
H	4.012161000	-3.374030000	-1.545187000
C	5.576018000	-4.073885000	1.901384000
H	4.188072000	-2.642842000	2.658282000
C	6.036723000	-4.734527000	0.782139000
H	6.836694000	-5.457256000	0.872940000
C	-4.571898000	-3.354428000	-2.271558000
H	-4.839401000	-3.104247000	-3.310126000
H	-3.742464000	-4.072804000	-2.362000000
Si	-6.119559000	-4.290736000	-1.646713000
C	-5.822875000	-5.374043000	-0.114683000
H	-4.972499000	-6.048794000	-0.269670000
H	-5.627385000	-4.784760000	0.785521000
H	-6.707121000	-5.995282000	0.074635000
C	-6.620342000	-5.461261000	-3.064986000
H	-5.820670000	-6.176423000	-3.293340000
H	-7.514936000	-6.037962000	-2.800921000
H	-6.842019000	-4.904751000	-3.983523000
C	-7.531071000	-3.064423000	-1.327473000
H	-7.232557000	-2.336913000	-0.565194000
H	-7.790045000	-2.515993000	-2.241110000
H	-8.433590000	-3.580663000	-0.979337000
N	-5.082603000	-1.945963000	1.119784000
C	-3.889745000	-2.525914000	0.924850000

C	-5.697535000	-2.135889000	2.291327000
C	-3.291642000	-3.322380000	1.913222000
C	-3.158836000	-2.258837000	-0.372826000
C	-5.177904000	-2.905603000	3.327749000
H	-6.665448000	-1.647888000	2.403130000
C	-3.940476000	-3.515373000	3.126296000
H	-2.327409000	-3.785531000	1.719598000
C	-4.073107000	-2.063348000	-1.592983000
H	-5.727476000	-3.026550000	4.256776000
H	-3.492875000	-4.134716000	3.899892000
H	-3.496801000	-1.492128000	-2.334900000
H	-4.920173000	-1.430365000	-1.308125000
C	-2.902705000	0.769728000	1.421559000
C	-4.073596000	1.302069000	2.039745000
C	-4.024342000	1.722321000	3.346670000
C	-2.809487000	1.657761000	4.064839000
C	-1.687940000	1.231544000	3.384685000
N	-1.703140000	0.836421000	2.096089000
H	-4.927292000	2.078593000	3.838310000
H	-5.005685000	1.295061000	1.482734000
H	-2.749353000	1.950746000	5.108008000
H	-0.711993000	1.211297000	3.863573000
C	-2.828919000	0.279450000	0.087142000
H	-3.737991000	0.441054000	-0.492094000
C	-2.168143000	-1.057964000	-0.200919000
H	-1.576796000	-1.045056000	-1.128797000
H	-1.462322000	-1.301591000	0.602306000
H	-2.517314000	-3.131592000	-0.568687000
C	-0.530237000	9.271081000	-0.083011000
H	0.264560000	9.473506000	-0.793954000
H	-1.421273000	9.802518000	-0.410334000
H	-0.236964000	9.683339000	0.880165000
C	-3.140288000	5.379050000	1.945421000
H	-3.831985000	4.728691000	1.416169000
H	-2.709340000	4.798308000	2.758419000
H	-3.701803000	6.201601000	2.377466000
C	7.443063000	0.636948000	-0.723394000
H	7.216418000	1.478165000	-0.075354000
H	7.268202000	-0.277918000	-0.167470000
H	8.497351000	0.679826000	-0.980445000
C	5.990848000	-5.231298000	-1.702377000
H	7.045291000	-5.020742000	-1.866394000
H	5.885303000	-6.305946000	-1.573210000
H	5.442269000	-4.938934000	-2.591689000

C	6.174588000	-4.343204000	3.280841000
H	5.409201000	-4.686352000	3.973001000
H	6.949377000	-5.100859000	3.225504000
H	6.611517000	-3.437450000	3.695185000
C	2.312615000	-1.302784000	1.720862000
C	3.160474000	-0.395466000	2.373089000
C	1.157087000	-1.690720000	2.380597000
C	2.884108000	0.081616000	3.640616000
H	4.068999000	-0.079956000	1.879907000
C	0.864851000	-1.238261000	3.671633000
H	0.466509000	-2.374137000	1.914044000
C	1.730464000	-0.357325000	4.291690000
H	1.517937000	-0.008170000	5.293443000
C	1.688687000	-2.750762000	-0.363837000
C	1.273177000	-3.930545000	0.270428000
C	1.234161000	-2.515751000	-1.650725000
C	0.404569000	-4.818448000	-0.333860000
H	1.664594000	-4.169789000	1.248497000
C	0.366014000	-3.406589000	-2.290349000
H	1.582574000	-1.649663000	-2.192904000
C	-0.050575000	-4.542475000	-1.623242000
H	-0.718038000	-5.238811000	-2.113292000
C	-0.372467000	-1.768638000	4.394063000
H	-0.575880000	-1.193207000	5.291135000
H	-1.245659000	-1.726120000	3.749915000
H	-0.224287000	-2.806666000	4.685917000
C	3.843005000	1.039462000	4.345826000
H	4.586639000	1.423442000	3.655000000
H	3.305768000	1.880152000	4.776896000
H	4.364979000	0.533514000	5.155618000
C	-0.029076000	-6.101419000	0.372699000
H	0.344911000	-6.128476000	1.390934000
H	-1.113200000	-6.179145000	0.402683000
H	0.349514000	-6.976086000	-0.151738000
C	-0.111533000	-3.133301000	-3.714940000
H	0.671355000	-2.661549000	-4.301342000
H	-0.400239000	-4.056377000	-4.207736000
H	-0.975667000	-2.472182000	-3.712925000

TS3^F_{iso}, $E_{\text{(SCF Done)}} = -3606.453691$ a.u. IF = $i239.18 \text{ cm}^{-1}$

Y	-1.024014000	-1.712517000	0.063485000
N	-3.510996000	-1.513761000	-0.904784000
C	-4.511471000	-1.228584000	0.141424000
H	-4.971574000	-2.176310000	0.436605000

H	-5.315278000	-0.582104000	-0.242879000
C	-3.874762000	-0.568725000	1.353235000
H	-3.424199000	0.388647000	1.096370000
H	-4.623099000	-0.401489000	2.139902000
O	-2.814193000	-1.380671000	1.872934000
C	-3.301416000	-2.443178000	2.697910000
H	-2.444717000	-3.043270000	2.998670000
H	-4.002605000	-3.083323000	2.155813000
H	-3.788896000	-2.016670000	3.584160000
O	-1.240918000	0.382707000	-0.422139000
C	-2.100800000	1.328089000	-0.778188000
C	-3.286960000	0.967243000	-1.462949000
C	-3.500671000	-0.444342000	-1.934464000
H	-4.458850000	-0.480703000	-2.482102000
H	-2.726586000	-0.723423000	-2.657635000
C	-1.892350000	2.711340000	-0.487578000
C	-2.904381000	3.614463000	-0.822344000
H	-2.759005000	4.651741000	-0.557733000
C	-4.098184000	3.267139000	-1.469216000
C	-4.253778000	1.921123000	-1.787787000
H	-5.140261000	1.574138000	-2.309012000
C	-0.592148000	3.179781000	0.277091000
C	-5.158291000	4.371193000	-1.795871000
C	-6.402153000	3.783907000	-2.512299000
H	-7.112936000	4.577922000	-2.719179000
H	-6.898025000	3.042364000	-1.894513000
H	-6.130517000	3.322524000	-3.456066000
C	-4.524312000	5.444080000	-2.725073000
H	-5.253932000	6.211476000	-2.966165000
H	-4.185429000	4.992548000	-3.652533000
H	-3.675235000	5.922478000	-2.248923000
O	-1.832799000	-3.681202000	0.204289000
C	-2.915730000	-4.424086000	0.072839000
C	-3.975273000	-4.012859000	-0.765082000
C	-3.823596000	-2.785150000	-1.619023000
H	-3.013536000	-2.932950000	-2.345232000
H	-4.748242000	-2.647590000	-2.206211000
C	-3.036728000	-5.650497000	0.778323000
C	-4.203860000	-6.399259000	0.648604000
H	-4.282797000	-7.336176000	1.195878000
C	-5.274464000	-5.992437000	-0.161647000
C	-5.132602000	-4.793698000	-0.859948000
H	-5.937892000	-4.455936000	-1.510580000
N	-0.107632000	-2.262811000	-2.213867000

C	-0.076644000	-3.625324000	-2.392867000
C	-0.503666000	-1.488222000	-3.251431000
C	-0.710974000	-4.198847000	-3.521403000
C	0.695739000	-4.411721000	-1.478178000
C	-0.991576000	-1.992718000	-4.441096000
H	-0.443839000	-0.417150000	-3.077980000
C	-1.149696000	-3.388964000	-4.548064000
H	-0.760472000	-5.281134000	-3.599080000
H	0.322975000	-5.395910000	-1.207546000
C	1.960626000	-4.016279000	-1.093267000
H	-1.280720000	-1.323681000	-5.245038000
H	-1.580233000	-3.826165000	-5.445538000
H	2.458533000	-3.247944000	-1.672682000
H	2.602242000	-4.754597000	-0.623777000
C	-0.627883000	4.728441000	0.532680000
C	-0.495920000	5.590604000	-0.567636000
C	-0.738894000	5.297580000	1.786912000
C	-0.490099000	6.962389000	-0.421241000
H	-0.396454000	5.167206000	-1.557354000
C	-0.733243000	6.686479000	1.963694000
H	-0.826140000	4.673377000	2.662638000
C	-0.612021000	7.506168000	0.861239000
H	-0.605725000	8.580871000	0.986027000
C	5.768651000	-0.717390000	-2.379660000
H	5.795488000	-1.138728000	-3.396394000
H	5.497173000	0.339308000	-2.524783000
Si	7.604641000	-0.801692000	-1.842080000
C	8.082098000	0.447661000	-0.493541000
H	7.778655000	1.462628000	-0.776908000
H	7.629118000	0.216506000	0.474512000
H	9.171381000	0.454088000	-0.362656000
C	8.611046000	-0.349488000	-3.395645000
H	8.363867000	0.657776000	-3.752487000
H	9.687229000	-0.371708000	-3.186305000
H	8.416695000	-1.050929000	-4.215849000
C	8.053367000	-2.565881000	-1.309122000
H	7.444233000	-2.867342000	-0.450818000
H	7.876726000	-3.280299000	-2.122186000
H	9.110408000	-2.635825000	-1.026208000
N	5.564304000	-1.649640000	1.145299000
C	4.849424000	-0.570327000	0.792825000
C	6.263569000	-1.607398000	2.283104000
C	4.837866000	0.588394000	1.581794000
C	3.999082000	-0.652494000	-0.459188000

C	6.302722000	-0.503819000	3.130592000
H	6.828835000	-2.506746000	2.526158000
C	5.570742000	0.623178000	2.762377000
H	4.256567000	1.449403000	1.264233000
C	4.645843000	-1.441623000	-1.609499000
H	6.892193000	-0.526982000	4.042555000
H	5.574907000	1.515842000	3.383179000
H	3.841949000	-1.658516000	-2.326812000
H	4.997604000	-2.409555000	-1.235619000
C	1.756478000	-2.782022000	1.688044000
C	2.139949000	-3.753975000	2.669829000
C	1.462409000	-3.870359000	3.852677000
C	0.361020000	-3.016538000	4.104181000
C	-0.032790000	-2.177637000	3.087381000
N	0.567227000	-2.089300000	1.873993000
H	1.789369000	-4.584698000	4.604976000
H	3.026365000	-4.351302000	2.474195000
H	-0.166291000	-3.022690000	5.052347000
H	-0.882162000	-1.515343000	3.226134000
C	2.566530000	-2.533458000	0.571293000
H	3.527522000	-3.038429000	0.605193000
C	2.576014000	-1.189934000	-0.111184000
H	2.007685000	-1.185241000	-1.059602000
H	2.080920000	-0.451319000	0.535665000
H	3.844005000	0.376156000	-0.814208000
C	-6.544545000	-6.847478000	-0.273136000
H	-7.259416000	-6.387348000	-0.947891000
H	-6.312731000	-7.841243000	-0.649965000
H	-7.021456000	-6.966544000	0.697435000
C	-1.874210000	-6.113294000	1.661744000
H	-0.949671000	-6.155011000	1.091469000
H	-1.711540000	-5.425826000	2.489241000
H	-2.072933000	-7.098676000	2.071539000
C	-5.631054000	5.046888000	-0.478044000
H	-6.079318000	4.314638000	0.186674000
H	-4.802462000	5.516304000	0.041246000
H	-6.372341000	5.811092000	-0.692040000
C	-0.350000000	7.884470000	-1.630810000
H	-1.216563000	8.535433000	-1.722119000
H	0.529010000	8.517285000	-1.532761000
H	-0.256464000	7.310145000	-2.546621000
C	-0.858468000	7.267394000	3.370985000
H	-0.051337000	6.912604000	4.007651000
H	-0.822889000	8.351615000	3.346788000

H	-1.797272000	6.966417000	3.830318000
C	-0.570513000	2.417714000	1.641932000
C	-1.755816000	2.374674000	2.390439000
C	0.560845000	1.832752000	2.188456000
C	-1.806819000	1.791668000	3.642746000
H	-2.648155000	2.831747000	1.986889000
C	0.536888000	1.243163000	3.457284000
H	1.491572000	1.836856000	1.643821000
C	-0.644995000	1.230967000	4.174417000
H	-0.671037000	0.784068000	5.159301000
C	0.700764000	2.958155000	-0.575052000
C	1.909887000	3.494734000	-0.113124000
C	0.692999000	2.374392000	-1.832197000
C	3.069040000	3.438141000	-0.865081000
H	1.933300000	3.996891000	0.843582000
C	1.851694000	2.297395000	-2.609041000
H	-0.229508000	1.999701000	-2.247237000
C	3.030465000	2.828020000	-2.118414000
H	3.929298000	2.786901000	-2.719251000
C	1.818693000	0.658428000	4.047238000
H	1.606366000	0.095509000	4.949985000
H	2.305390000	-0.002162000	3.335746000
H	2.518755000	1.452825000	4.298331000
C	-3.099694000	1.788107000	4.456755000
H	-3.940191000	2.114599000	3.852912000
H	-3.314958000	0.793752000	4.839211000
H	-3.017748000	2.457507000	5.310694000
C	4.364619000	4.071709000	-0.360999000
H	4.296427000	4.307069000	0.696161000
H	5.208582000	3.404164000	-0.512630000
H	4.572425000	4.994625000	-0.898921000
C	1.813751000	1.637355000	-3.986303000
H	0.834685000	1.747964000	-4.442813000
H	2.553696000	2.078425000	-4.647243000
H	2.029762000	0.573371000	-3.908173000

P3^F_{iso}, $E_{(\text{SCF Done})} = -3606.502875$ a.u.

Y	0.415310000	1.972465000	-0.078040000
N	2.769520000	2.817716000	-0.864268000
C	3.764269000	2.953711000	0.217056000
H	3.806500000	4.008036000	0.507072000
H	4.768830000	2.670579000	-0.132331000
C	3.403037000	2.103931000	1.424501000
H	3.382985000	1.044592000	1.175382000

H	4.128865000	2.260613000	2.235011000
O	2.087397000	2.420400000	1.895660000
C	2.063252000	3.591244000	2.710881000
H	1.023204000	3.788043000	2.969080000
H	2.452571000	4.464596000	2.180555000
H	2.649110000	3.414217000	3.623299000
O	1.547118000	0.110530000	-0.336173000
C	2.704588000	-0.373172000	-0.737988000
C	3.628076000	0.465501000	-1.415768000
C	3.218935000	1.835691000	-1.885198000
H	4.067433000	2.275441000	-2.438144000
H	2.395512000	1.746142000	-2.600559000
C	3.086464000	-1.733766000	-0.518827000
C	4.375578000	-2.130076000	-0.881629000
H	4.669177000	-3.147984000	-0.666286000
C	5.317122000	-1.294610000	-1.498676000
C	4.898887000	0.006278000	-1.768064000
H	5.556575000	0.703721000	-2.277633000
C	2.092700000	-2.724822000	0.204867000
C	6.737531000	-1.848045000	-1.852949000
C	7.626233000	-0.770774000	-2.527742000
H	8.602401000	-1.189716000	-2.751846000
H	7.769792000	0.084706000	-1.875835000
H	7.187335000	-0.426367000	-3.458350000
C	6.603261000	-3.048149000	-2.831944000
H	7.584347000	-3.435063000	-3.091430000
H	6.105742000	-2.739547000	-3.746322000
H	6.028926000	-3.853785000	-2.387400000
O	0.306551000	4.116302000	0.196258000
C	1.004384000	5.227498000	0.089004000
C	2.170543000	5.287786000	-0.709845000
C	2.560543000	4.116181000	-1.569206000
H	1.784949000	3.932880000	-2.324897000
H	3.481166000	4.374744000	-2.121400000
C	0.595209000	6.400339000	0.780076000
C	1.361968000	7.558655000	0.686468000
H	1.030929000	8.446342000	1.221920000
C	2.535675000	7.622842000	-0.079281000
C	2.913807000	6.471936000	-0.770467000
H	3.808393000	6.493047000	-1.391482000
N	-0.338363000	1.968715000	-2.486397000
C	-1.434490000	2.665019000	-2.025862000
C	0.170491000	2.284589000	-3.695638000
C	-1.840840000	3.856306000	-2.704030000

C	-2.005151000	2.164401000	-0.837238000
C	-0.264332000	3.346964000	-4.458846000
H	0.971330000	1.639343000	-4.053447000
C	-1.268570000	4.178266000	-3.908917000
H	-2.636371000	4.459772000	-2.276070000
H	-2.780236000	2.781349000	-0.384138000
C	-2.186680000	0.668716000	-0.647975000
H	0.166836000	3.544288000	-5.434822000
H	-1.604643000	5.057837000	-4.453762000
H	-1.246838000	0.092512000	-0.526788000
H	-2.652094000	0.205466000	-1.529793000
C	2.747307000	-4.143544000	0.352517000
C	2.919537000	-4.923446000	-0.801804000
C	3.143897000	-4.684350000	1.560967000
C	3.471563000	-6.186965000	-0.750531000
H	2.612925000	-4.521125000	-1.757312000
C	3.704199000	-5.964621000	1.641104000
H	3.022439000	-4.123522000	2.474781000
C	3.864496000	-6.703882000	0.487819000
H	4.295772000	-7.694866000	0.537879000
C	-6.067636000	-2.165708000	-2.004517000
H	-5.770620000	-2.287774000	-3.057046000
H	-6.066883000	-3.188199000	-1.596897000
Si	-7.879846000	-1.562467000	-2.147649000
C	-8.947620000	-1.922252000	-0.617958000
H	-8.879715000	-2.978480000	-0.331322000
H	-8.662786000	-1.317294000	0.247509000
H	-9.999708000	-1.709063000	-0.844317000
C	-8.634124000	-2.541694000	-3.595626000
H	-8.600953000	-3.621680000	-3.407251000
H	-9.683463000	-2.264738000	-3.752113000
H	-8.095676000	-2.349622000	-4.531258000
C	-7.917276000	0.288631000	-2.558423000
H	-7.457392000	0.871572000	-1.753404000
H	-7.369249000	0.498158000	-3.484691000
H	-8.947199000	0.639993000	-2.692444000
N	-6.302351000	0.274767000	0.782382000
C	-5.886646000	-0.970344000	1.062062000
C	-7.208397000	0.841381000	1.585968000
C	-6.382550000	-1.676952000	2.167608000
C	-4.797233000	-1.567824000	0.192777000
C	-7.749906000	0.215792000	2.706223000
H	-7.517004000	1.850265000	1.314895000
C	-7.322654000	-1.078406000	2.998838000

H	-6.030414000	-2.686087000	2.365646000
C	-4.975307000	-1.323884000	-1.314027000
H	-8.485862000	0.724800000	3.321670000
H	-7.720432000	-1.614287000	3.857166000
H	-4.013634000	-1.569467000	-1.783321000
H	-5.139532000	-0.254932000	-1.491193000
C	-2.438626000	0.907933000	1.855322000
C	-3.258357000	1.054491000	2.983332000
C	-2.714446000	1.437000000	4.200752000
C	-1.338088000	1.630432000	4.280470000
C	-0.590089000	1.478402000	3.120988000
N	-1.115712000	1.168899000	1.920454000
H	-3.349235000	1.564776000	5.073888000
H	-4.322475000	0.861990000	2.885794000
H	-0.849153000	1.895115000	5.212707000
H	0.487133000	1.598673000	3.137397000
C	-3.056725000	0.386783000	0.573106000
H	-4.003465000	0.929033000	0.444346000
C	-3.403378000	-1.123628000	0.718177000
H	-2.636941000	-1.713889000	0.198507000
H	-3.348183000	-1.418024000	1.773474000
H	-4.826379000	-2.655719000	0.353974000
C	3.356214000	8.918253000	-0.155365000
H	4.210235000	8.793641000	-0.813584000
H	2.753053000	9.740298000	-0.534508000
H	3.724873000	9.207028000	0.826819000
C	-0.697362000	6.349454000	1.600998000
H	-1.514583000	5.955201000	1.001885000
H	-0.589610000	5.700616000	2.468227000
H	-0.970343000	7.339916000	1.952041000
C	7.452228000	-2.322007000	-0.556051000
H	7.560432000	-1.497909000	0.142626000
H	6.892721000	-3.111920000	-0.066557000
H	8.442267000	-2.703251000	-0.788360000
C	3.654741000	-7.019916000	-2.017636000
H	4.703921000	-7.261455000	-2.172125000
H	3.107680000	-7.957063000	-1.945029000
H	3.296381000	-6.482214000	-2.889262000
C	4.125608000	-6.519344000	3.000694000
H	3.278302000	-6.557226000	3.681413000
H	4.528869000	-7.521848000	2.901805000
H	4.885963000	-5.888715000	3.455777000
C	1.803184000	-2.139770000	1.628400000
C	2.872895000	-1.590321000	2.349481000

C	0.572939000	-2.215861000	2.265173000
C	2.729171000	-1.149260000	3.652549000
H	3.844821000	-1.531178000	1.881074000
C	0.408646000	-1.800516000	3.589108000
H	-0.282178000	-2.621336000	1.748915000
C	1.486058000	-1.268709000	4.272514000
H	1.368148000	-0.948428000	5.299127000
C	0.792123000	-2.968441000	-0.631379000
C	-0.097649000	-3.974332000	-0.223041000
C	0.521089000	-2.318853000	-1.823384000
C	-1.229609000	-4.287071000	-0.949279000
H	0.118779000	-4.540747000	0.671119000
C	-0.619770000	-2.615541000	-2.577864000
H	1.205409000	-1.579395000	-2.208110000
C	-1.489136000	-3.590571000	-2.131587000
H	-2.370947000	-3.832843000	-2.709690000
C	-0.938187000	-1.994115000	4.283892000
H	-0.998439000	-1.399571000	5.189628000
H	-1.759184000	-1.714452000	3.631160000
H	-1.076436000	-3.038264000	4.558392000
C	3.916071000	-0.573926000	4.423598000
H	4.782965000	-0.469144000	3.779434000
H	3.674325000	0.402554000	4.836065000
H	4.187226000	-1.222890000	5.253601000
C	-2.177875000	-5.393317000	-0.490377000
H	-1.887715000	-5.773751000	0.483575000
H	-3.199099000	-5.025961000	-0.424956000
H	-2.171342000	-6.222786000	-1.194263000
C	-0.870027000	-1.870671000	-3.887603000
H	-0.068283000	-2.062884000	-4.597106000
H	-1.806119000	-2.183530000	-4.338513000
H	-0.910880000	-0.797729000	-3.716260000

TS2^A_{syn} $E_{(\text{SCF Done})} = -3472.499785$ a.u. IF = $i210.51$ cm⁻¹

Y	0.029896000	0.870361000	0.406775000
N	0.215875000	-1.645504000	0.443304000
C	0.033439000	-2.229755000	-0.898829000
H	-1.038693000	-2.353182000	-1.065490000
H	0.496717000	-3.226893000	-0.963281000
C	0.595603000	-1.367311000	-2.019811000
H	1.689018000	-1.318283000	-2.007482000
H	0.273445000	-1.797805000	-2.979033000
O	0.060680000	-0.044404000	-1.907337000
C	0.194239000	0.716698000	-3.099167000

H	-0.257080000	1.692391000	-2.910059000
H	-0.340549000	0.224637000	-3.921512000
H	1.250300000	0.837303000	-3.373414000
O	2.190914000	0.524541000	0.184939000
C	3.100704000	-0.430126000	-0.005976000
C	2.757075000	-1.769191000	0.303578000
C	1.496070000	-2.062819000	1.063533000
H	1.449579000	-3.148236000	1.255356000
H	1.526722000	-1.580621000	2.049608000
C	4.417431000	-0.192644000	-0.509115000
C	5.198761000	-1.300476000	-0.851019000
H	6.172708000	-1.112953000	-1.289034000
C	4.823436000	-2.634181000	-0.645030000
C	3.594335000	-2.837225000	-0.025207000
H	3.255100000	-3.837869000	0.224051000
C	4.985230000	1.250703000	-0.768608000
C	5.773793000	-3.782762000	-1.125122000
O	-2.020656000	0.156603000	0.161791000
C	-2.762610000	-0.946373000	0.180812000
C	-2.250173000	-2.075566000	0.867084000
C	-0.860305000	-2.023532000	1.419284000
H	-0.781853000	-1.299506000	2.247146000
H	-0.618125000	-3.006701000	1.851710000
C	-4.034602000	-1.094538000	-0.452545000
C	-4.761918000	-2.261411000	-0.191136000
H	-5.759265000	-2.331914000	-0.612519000
C	-4.297731000	-3.344339000	0.563594000
C	-2.998240000	-3.238938000	1.049547000
H	-2.537863000	-4.057273000	1.594371000
C	5.798944000	-3.760369000	-2.679835000
H	4.785735000	-3.851418000	-3.059093000
H	6.218995000	-2.833406000	-3.055204000
H	6.379414000	-4.588143000	-3.074051000
C	-3.804547000	4.908706000	-0.022646000
H	-4.670638000	4.587902000	-0.622011000
H	-4.212856000	5.146130000	0.971659000
Si	-3.174723000	6.524549000	-0.824534000
C	-2.060387000	7.531973000	0.336329000
H	-2.566204000	7.742678000	1.286286000
H	-1.130620000	6.997217000	0.556760000
H	-1.797064000	8.493657000	-0.120861000
C	-4.697769000	7.579936000	-1.258340000
H	-5.286637000	7.814934000	-0.363582000
H	-4.399037000	8.529263000	-1.718637000

H	-5.355810000	7.058948000	-1.963834000
C	-2.225610000	6.114558000	-2.418793000
H	-1.335131000	5.514736000	-2.198870000
H	-2.852771000	5.547504000	-3.117376000
H	-1.898499000	7.028671000	-2.928258000
N	0.088943000	3.191213000	-0.347779000
C	-0.368883000	3.982171000	0.711619000
C	1.237932000	3.578720000	-0.960597000
C	0.567109000	4.866271000	1.347739000
C	-1.721051000	3.954889000	1.096393000
C	2.060322000	4.587478000	-0.519887000
H	1.505935000	3.004043000	-1.842736000
C	1.745468000	5.184708000	0.726702000
H	0.269802000	5.350557000	2.274242000
C	-2.820612000	3.726233000	0.088412000
H	2.954285000	4.854284000	-1.072311000
H	2.421556000	5.910176000	1.173154000
H	-3.399339000	2.825016000	0.324308000
H	-2.362600000	3.528802000	-0.888687000
C	6.540456000	1.242119000	-0.811362000
C	7.252490000	0.806230000	0.311414000
C	7.272985000	1.696074000	-1.900553000
C	8.632925000	0.822564000	0.340444000
H	6.712754000	0.437042000	1.172792000
C	8.662870000	1.715550000	-1.874944000
H	6.772798000	2.045076000	-2.791095000
C	9.349001000	1.281170000	-0.758073000
H	10.430850000	1.295931000	-0.737935000
C	-0.237672000	1.685862000	3.939833000
C	0.307921000	1.708044000	5.252548000
C	1.586142000	1.271327000	5.505157000
C	2.362611000	0.821192000	4.426407000
C	1.783027000	0.807734000	3.173174000
N	0.510228000	1.187854000	2.896154000
H	1.988614000	1.291762000	6.514984000
H	-0.317145000	2.088721000	6.055282000
H	3.391195000	0.499133000	4.550114000
H	2.366929000	0.502324000	2.313169000
C	-1.537966000	2.243173000	3.755169000
H	-1.916472000	2.795867000	4.612956000
C	-2.270179000	2.274264000	2.596367000
H	-1.955638000	4.660703000	1.890656000
C	5.262218000	-5.183366000	-0.682831000
H	5.170441000	-5.248367000	0.396033000

H	4.296060000	-5.401146000	-1.126529000
H	5.962117000	-5.946734000	-1.009026000
C	-4.730854000	-0.003943000	-1.346296000
C	-5.206964000	-4.607219000	0.737370000
H	-3.261251000	2.717907000	2.627324000
H	-2.168066000	1.533253000	1.809375000
C	-5.554539000	0.914503000	-0.401719000
H	-4.907622000	1.305711000	0.375548000
H	-5.983571000	1.753793000	-0.939641000
H	-6.355394000	0.359894000	0.076579000
C	-3.704191000	0.861188000	-2.129960000
H	-3.079624000	1.422416000	-1.452277000
H	-3.067168000	0.236979000	-2.746504000
H	-4.229655000	1.556753000	-2.777450000
C	-5.284172000	-5.335440000	-0.634395000
H	-5.839382000	-6.264452000	-0.554429000
H	-5.756946000	-4.712147000	-1.385995000
H	-4.280696000	-5.573062000	-0.973880000
C	-4.617734000	-5.607300000	1.772941000
H	-3.672336000	-6.012460000	1.427263000
H	-4.459031000	-5.130947000	2.734611000
H	-5.305983000	-6.435285000	1.913728000
C	-6.604384000	-4.164133000	1.252290000
C	-7.796391000	-4.581517000	0.673949000
C	-6.677995000	-3.333274000	2.373265000
C	-9.021658000	-4.181009000	1.192673000
H	-7.789092000	-5.224984000	-0.193149000
C	-7.894652000	-2.933802000	2.892243000
H	-5.764043000	-2.990114000	2.839716000
C	-9.077550000	-3.357882000	2.301349000
H	-9.935865000	-4.518784000	0.721110000
H	-7.923739000	-2.287725000	3.760527000
H	-10.032071000	-3.045705000	2.704528000
C	-5.627377000	-0.682754000	-2.422614000
C	-6.964695000	-0.360111000	-2.613155000
C	-5.058745000	-1.626025000	-3.284998000
C	-7.711062000	-0.958116000	-3.622313000
H	-7.449528000	0.364347000	-1.976277000
C	-5.796639000	-2.222928000	-4.287857000
H	-4.020605000	-1.901765000	-3.157617000
C	-7.133859000	-1.889701000	-4.462779000
H	-8.752145000	-0.687477000	-3.745634000
H	-5.330822000	-2.952266000	-4.938407000
H	-7.714996000	-2.355426000	-5.247847000

C	7.184622000	-3.578302000	-0.506807000
C	8.355646000	-3.615141000	-1.253084000
C	7.294758000	-3.384576000	0.872397000
C	9.595740000	-3.460671000	-0.645670000
H	8.320114000	-3.763777000	-2.322020000
C	8.526329000	-3.232018000	1.479962000
H	6.397362000	-3.347463000	1.475614000
C	9.687837000	-3.269670000	0.719985000
H	10.492968000	-3.491220000	-1.250918000
H	8.583903000	-3.082085000	2.550659000
H	10.653982000	-3.149484000	1.192491000
H	9.205750000	2.075622000	-2.739716000
H	9.156581000	0.475243000	1.222021000
C	4.376155000	1.758698000	-2.103443000
H	4.663684000	2.785308000	-2.305679000
H	4.689715000	1.138003000	-2.936569000
H	3.295766000	1.716329000	-2.039279000
C	4.582082000	2.227467000	0.374245000
H	4.915236000	1.854762000	1.336241000
H	5.039783000	3.197660000	0.207880000
H	3.509030000	2.352526000	0.408011000

TS2^A_{iso}, $E_{\text{(SCF Done)}} = -3472.499661$ a.u. **IF** = $i202.76$ cm⁻¹

Y	-0.019444000	0.464077000	0.287874000
N	-0.051815000	-2.070036000	-0.064357000
C	0.122496000	-2.799754000	1.205408000
H	1.195103000	-2.937130000	1.374645000
H	-0.335415000	-3.800361000	1.154225000
C	-0.483817000	-2.025480000	2.362888000
H	-1.552519000	-1.864264000	2.212362000
H	-0.337158000	-2.558179000	3.310978000
O	0.108754000	-0.719379000	2.457181000
C	1.264346000	-0.652678000	3.291211000
H	1.559421000	0.395917000	3.338789000
H	2.089767000	-1.244582000	2.881099000
H	1.010824000	-1.003667000	4.298573000
O	-2.104715000	0.008216000	0.246397000
C	-3.061442000	-0.932201000	0.244263000
C	-2.637108000	-2.251191000	-0.047612000
C	-1.320139000	-2.464625000	-0.743306000
H	-1.234666000	-3.530861000	-1.011600000
H	-1.324128000	-1.912827000	-1.693825000
C	-4.443537000	-0.695880000	0.532710000
C	-5.239536000	-1.837533000	0.647349000

H	-6.291290000	-1.668746000	0.862731000
C	-4.814945000	-3.163178000	0.501006000
C	-3.492522000	-3.341801000	0.102472000
H	-3.110009000	-4.329821000	-0.136316000
C	-5.111249000	0.720647000	0.656176000
C	-5.819546000	-4.331397000	0.779513000
O	2.089164000	0.016408000	0.042334000
C	2.940456000	-1.004393000	-0.053439000
C	2.453520000	-2.245343000	-0.526903000
C	1.046035000	-2.355742000	-1.036080000
H	0.895912000	-1.657949000	-1.874511000
H	0.900960000	-3.368355000	-1.446282000
C	4.330411000	-0.910300000	0.273827000
C	5.116062000	-2.053026000	0.113908000
H	6.175716000	-1.973375000	0.322142000
C	4.636986000	-3.296649000	-0.322062000
C	3.285486000	-3.363803000	-0.637187000
H	2.844814000	-4.285146000	-1.004748000
C	-6.121346000	-4.340213000	2.305063000
H	-5.190581000	-4.424743000	2.857601000
H	-6.617071000	-3.426315000	2.614476000
H	-6.748789000	-5.183295000	2.575340000
C	-0.156629000	6.334235000	-0.074672000
H	-0.945061000	6.636239000	0.631004000
H	0.732190000	6.147080000	0.539051000
Si	0.160332000	7.888957000	-1.139791000
C	1.737386000	7.770812000	-2.199003000
H	2.603787000	7.471639000	-1.597340000
H	1.628807000	7.050905000	-3.017874000
H	1.965244000	8.745660000	-2.647201000
C	0.366616000	9.349162000	0.060996000
H	1.213683000	9.189433000	0.738896000
H	0.547250000	10.284283000	-0.482149000
H	-0.531147000	9.487253000	0.674933000
C	-1.324313000	8.213583000	-2.279089000
H	-1.451185000	7.408662000	-3.012129000
H	-2.255873000	8.293973000	-1.706759000
H	-1.190697000	9.149735000	-2.834091000
N	-0.383872000	2.023717000	-1.673043000
C	0.384586000	3.073068000	-2.167245000
C	-0.675071000	1.009196000	-2.529038000
C	1.105644000	2.863098000	-3.391180000
C	0.480798000	4.324558000	-1.531035000
C	-0.108382000	0.829038000	-3.773288000

H	-1.421678000	0.305581000	-2.156909000
C	0.866124000	1.768989000	-4.181642000
H	1.798803000	3.635500000	-3.714696000
C	-0.609418000	5.038205000	-0.776520000
H	-0.397984000	-0.009008000	-4.398685000
H	1.390052000	1.648158000	-5.126492000
H	-1.092326000	4.363537000	-0.062091000
H	-1.402671000	5.340225000	-1.495362000
C	-6.460825000	0.705753000	-0.118385000
C	-6.458228000	0.340695000	-1.468000000
C	-7.671319000	1.081305000	0.448912000
C	-7.619066000	0.348733000	-2.216297000
H	-5.529323000	0.040628000	-1.934562000
C	-8.841638000	1.089731000	-0.301049000
H	-7.723692000	1.374349000	1.486666000
C	-8.822380000	0.725247000	-1.633251000
H	-9.733629000	0.732006000	-2.216884000
C	0.425844000	3.380199000	2.366472000
C	0.096850000	4.079560000	3.551505000
C	-0.969705000	3.686370000	4.334363000
C	-1.734768000	2.588427000	3.927194000
C	-1.355894000	1.929495000	2.770135000
N	-0.295287000	2.274362000	2.008770000
H	-1.218319000	4.233434000	5.240324000
H	0.693482000	4.945391000	3.823452000
H	-2.606486000	2.255988000	4.480381000
H	-1.935807000	1.084577000	2.410882000
C	1.502766000	3.897465000	1.559152000
H	1.963332000	4.794564000	1.967743000
C	1.918496000	3.479148000	0.332489000
H	2.778944000	3.948668000	-0.132134000
H	1.662540000	2.515581000	-0.084869000
H	1.197519000	4.990041000	-2.011754000
C	-5.215474000	-5.716220000	0.410499000
H	-4.936524000	-5.759474000	-0.636849000
H	-4.337915000	-5.929616000	1.012309000
H	-5.949087000	-6.494678000	0.596946000
C	5.001942000	0.462827000	0.656958000
C	5.624142000	-4.510256000	-0.398155000
C	4.895582000	1.383804000	-0.590337000
H	3.852617000	1.503122000	-0.859636000
H	5.313199000	2.364969000	-0.388392000
H	5.413751000	0.951737000	-1.439549000
C	4.259545000	1.152158000	1.839072000

H	3. 251091000	1. 413165000	1. 552297000
H	4. 214451000	0. 505509000	2. 707335000
H	4. 780024000	2. 062393000	2. 120693000
C	5. 996502000	-4. 912226000	1. 057211000
H	6. 616839000	-5. 802469000	1. 071252000
H	6. 526331000	-4. 112748000	1. 564135000
H	5. 090739000	-5. 126699000	1. 616127000
C	4. 972750000	-5. 747678000	-1. 078903000
H	4. 130226000	-6. 111246000	-0. 499561000
H	4. 628598000	-5. 511563000	-2. 080188000
H	5. 701497000	-6. 549320000	-1. 151614000
C	6. 867911000	-4. 108848000	-1. 238484000
C	8. 173413000	-4. 324939000	-0. 816072000
C	6. 674714000	-3. 534880000	-2. 497522000
C	9. 251769000	-3. 976396000	-1. 619972000
H	8. 371439000	-4. 767318000	0. 148828000
C	7. 744794000	-3. 187744000	-3. 299869000
H	5. 667663000	-3. 351844000	-2. 848260000
C	9. 044178000	-3. 407933000	-2. 862448000
H	10. 259475000	-4. 153201000	-1. 265717000
H	7. 567679000	-2. 741997000	-4. 270519000
H	9. 884450000	-3. 135868000	-3. 487823000
C	6. 481117000	0. 275041000	1. 104257000
C	7. 557734000	0. 783717000	0. 387700000
C	6. 763129000	-0. 403261000	2. 295209000
C	8. 862783000	0. 628201000	0. 840010000
H	7. 397862000	1. 313043000	-0. 539239000
C	8. 058495000	-0. 561654000	2. 747694000
H	5. 953515000	-0. 826279000	2. 873273000
C	9. 120670000	-0. 041861000	2. 020050000
H	9. 679202000	1. 037751000	0. 258666000
H	8. 243672000	-1. 093440000	3. 672344000
H	10. 136607000	-0. 162703000	2. 372673000
C	-7. 100502000	-4. 131088000	-0. 076842000
C	-8. 384981000	-4. 205773000	0. 446603000
C	-6. 965774000	-3. 902390000	-1. 448387000
C	-9. 499241000	-4. 053490000	-0. 369301000
H	-8. 538129000	-4. 382875000	1. 500701000
C	-8. 071720000	-3. 751609000	-2. 262961000
H	-5. 976035000	-3. 835204000	-1. 880234000
C	-9. 349361000	-3. 826828000	-1. 724378000
H	-10. 489456000	-4. 113801000	0. 064371000
H	-7. 939739000	-3. 573012000	-3. 322620000
H	-10. 217589000	-3. 707617000	-2. 359310000

C	-5.311668000	1.022216000	2.168645000
H	-5.720254000	2.016216000	2.319876000
H	-5.976062000	0.299155000	2.630426000
H	-4.354820000	0.972390000	2.677773000
C	-4.261248000	1.869856000	0.041132000
H	-3.374005000	2.062705000	0.629234000
H	-3.955468000	1.637768000	-0.972477000
H	-4.856309000	2.778237000	0.018170000
H	-9.771892000	1.385580000	0.167258000
H	-7.589143000	0.060506000	-3.259446000

TS2^c_{syn}, $E_{(\text{SCF Done})} = -3089.24034 \text{ a.u.}$ IF = $i171.98 \text{ cm}^{-1}$

Y	0.976892000	-0.246168000	0.346591000
N	0.154112000	2.179420000	0.101824000
C	0.275318000	2.641428000	-1.293167000
H	1.297996000	2.999004000	-1.444550000
H	-0.401269000	3.488310000	-1.492105000
C	-0.020746000	1.518205000	-2.273863000
H	-1.035992000	1.138551000	-2.154739000
H	0.101810000	1.870822000	-3.305729000
O	0.857937000	0.406334000	-2.044348000
C	2.016913000	0.393516000	-2.876959000
H	2.567269000	-0.514528000	-2.630013000
H	2.648172000	1.269159000	-2.693090000
H	1.711902000	0.362338000	-3.930146000
O	-1.180933000	-0.417024000	0.155070000
C	-2.321433000	0.202124000	-0.128991000
C	-2.348871000	1.619397000	-0.067999000
C	-1.229116000	2.355120000	0.609758000
H	-1.462484000	3.433269000	0.594218000
H	-1.193059000	2.074129000	1.670627000
C	-3.530660000	-0.457985000	-0.493127000
C	-4.591667000	0.329427000	-0.958795000
H	-5.490969000	-0.186990000	-1.279993000
C	-4.585213000	1.727200000	-1.015603000
C	-3.444049000	2.354902000	-0.520909000
H	-3.384678000	3.437475000	-0.462701000
C	-3.758238000	-2.013292000	-0.482076000
C	-5.814893000	2.480318000	-1.626761000
O	2.849757000	0.942677000	0.388711000
C	3.304191000	2.198102000	0.316018000
C	2.404197000	3.254090000	0.585778000
C	1.020680000	2.942409000	1.053784000
H	1.051037000	2.348022000	1.980850000

H	0.516926000	3.887741000	1.309918000
C	4.651849000	2.565807000	-0.014475000
C	4.958319000	3.924516000	-0.115390000
H	5.970599000	4.193304000	-0.377962000
C	4.056373000	4.974869000	0.109102000
C	2.771388000	4.598545000	0.476143000
H	2.013004000	5.342839000	0.695734000
C	-5.849936000	2.171450000	-3.150466000
H	-4.902401000	2.454476000	-3.598539000
H	-6.009466000	1.114633000	-3.335666000
H	-6.635582000	2.732537000	-3.646006000
C	5.506924000	-3.586775000	-0.284247000
H	6.367834000	-3.030414000	-0.686601000
H	5.841586000	-3.968437000	0.692690000
Si	5.251484000	-5.071907000	-1.460289000
C	4.242638000	-6.475160000	-0.675018000
H	4.679238000	-6.789079000	0.280637000
H	3.207563000	-6.168089000	-0.493310000
H	4.224271000	-7.350083000	-1.336352000
C	6.978321000	-5.747728000	-1.889670000
H	7.510646000	-6.075485000	-0.988571000
H	6.909527000	-6.608341000	-2.565698000
H	7.593986000	-4.985023000	-2.381198000
C	4.396117000	-4.486271000	-3.051909000
H	3.382517000	-4.127445000	-2.840487000
H	4.955375000	-3.669666000	-3.524405000
H	4.317311000	-5.302600000	-3.779609000
N	1.423213000	-2.359267000	-0.753921000
C	1.915736000	-3.328897000	0.124038000
C	0.471509000	-2.747563000	-1.644284000
C	1.115963000	-4.498359000	0.351744000
C	3.188203000	-3.190607000	0.699039000
C	-0.137429000	-3.980163000	-1.638418000
H	0.176843000	-1.985405000	-2.361880000
C	0.138525000	-4.839592000	-0.544573000
H	1.389857000	-5.162257000	1.167632000
C	4.337794000	-2.601205000	-0.081995000
H	-0.865631000	-4.242120000	-2.397185000
H	-0.407735000	-5.773084000	-0.430856000
H	4.741820000	-1.702906000	0.399811000
H	3.961802000	-2.263386000	-1.055879000
C	-5.210247000	-2.321973000	-0.014945000
C	-5.651564000	-1.808967000	1.208675000
C	-6.083990000	-3.132093000	-0.728474000

C	-6.913376000	-2.091113000	1.694018000
H	-4.993736000	-1.171230000	1.783783000
C	-7.354848000	-3.418155000	-0.243438000
H	-5.788318000	-3.554878000	-1.676853000
C	-7.775591000	-2.901526000	0.966529000
H	-8.765112000	-3.123937000	1.343792000
C	1.172795000	-1.390670000	3.807573000
C	0.585078000	-1.592837000	5.084743000
C	-0.674958000	-1.125077000	5.374514000
C	-1.387616000	-0.462390000	4.365177000
C	-0.776881000	-0.314123000	3.135061000
N	0.472561000	-0.732754000	2.824946000
H	-1.109523000	-1.277964000	6.359288000
H	1.166207000	-2.122368000	5.834196000
H	-2.396760000	-0.094313000	4.517273000
H	-1.331899000	0.127677000	2.318304000
C	2.487078000	-1.908708000	3.593994000
H	2.844871000	-2.579299000	4.372775000
C	3.290254000	-1.695110000	2.508201000
H	3.453963000	-4.007394000	1.368585000
C	-5.692895000	4.022072000	-1.461675000
H	-5.609195000	4.302683000	-0.417226000
H	-4.825972000	4.401478000	-1.992933000
H	-6.575800000	4.503528000	-1.871167000
C	5.780232000	1.494609000	-0.200168000
C	4.527382000	6.459596000	-0.037369000
H	4.315447000	-2.047568000	2.541110000
H	3.148627000	-0.847563000	1.843700000
C	5.939388000	0.716805000	1.133512000
H	4.992416000	0.297358000	1.445250000
H	6.659467000	-0.088345000	1.024516000
H	6.289863000	1.384378000	1.914750000
C	5.408378000	0.536220000	-1.360536000
H	4.452139000	0.068934000	-1.174633000
H	5.351923000	1.085367000	-2.295441000
H	6.157996000	-0.241092000	-1.468203000
C	5.037773000	6.704874000	-1.485133000
H	5.361745000	7.734935000	-1.600658000
H	5.876830000	6.058901000	-1.720100000
H	4.248288000	6.513610000	-2.205621000
C	3.376755000	7.459991000	0.246349000
H	2.551366000	7.314882000	-0.442970000
H	3.004263000	7.352645000	1.259764000
H	3.738830000	8.476516000	0.127704000

C	-7.112410000	2.028904000	-0.900849000
C	-8.257768000	1.620639000	-1.572455000
C	-7.152599000	2.067787000	0.495095000
C	-9.404579000	1.259499000	-0.876048000
H	-8.274219000	1.576156000	-2.651206000
C	-8.291772000	1.710830000	1.190834000
H	-6.272114000	2.377655000	1.042147000
C	-9.428250000	1.303165000	0.505065000
H	-10.283054000	0.942693000	-1.423931000
H	-8.296145000	1.748513000	2.272825000
H	-10.321640000	1.021512000	1.046957000
H	-8.015394000	-4.051476000	-0.822109000
H	-7.230166000	-1.678290000	2.643388000
C	-3.484526000	-2.534949000	-1.919654000
H	-3.549287000	-3.617127000	-1.965788000
H	-4.189133000	-2.113290000	-2.629155000
H	-2.484255000	-2.244366000	-2.222070000
C	-2.818721000	-2.761335000	0.506399000
H	-2.871945000	-2.327262000	1.498614000
H	-3.121496000	-3.802116000	0.573964000
H	-1.792995000	-2.727479000	0.167539000
C	5.677645000	6.744239000	0.968778000
H	5.342586000	6.576184000	1.987775000
H	6.531026000	6.101673000	0.780773000
H	6.005793000	7.775950000	0.883290000
C	7.161485000	2.116373000	-0.541818000
H	7.131094000	2.670434000	-1.474116000
H	7.509345000	2.777014000	0.244993000
H	7.889454000	1.318526000	-0.652128000

TS2^c_{iso}, $E_{\text{(SCF Done)}} = -3089.232208 \text{ a.u.}$ IF = *i*198.78 cm⁻¹

Y	1.012018000	-0.086296000	0.192183000
N	0.157412000	-2.455830000	-0.326208000
C	0.073142000	-3.295654000	0.883730000
H	1.027512000	-3.817352000	1.005281000
H	-0.712990000	-4.060020000	0.782064000
C	-0.202694000	-2.444418000	2.109756000
H	-1.149562000	-1.910394000	2.012515000
H	-0.235000000	-3.058689000	3.018494000
O	0.812493000	-1.437906000	2.253511000
C	1.940675000	-1.838237000	3.030843000
H	2.568584000	-0.955419000	3.155082000
H	2.514375000	-2.626464000	2.531158000
H	1.603668000	-2.182326000	4.015806000

O	-1.113199000	0.142614000	0.192578000
C	-2.319811000	-0.442401000	0.161417000
C	-2.342843000	-1.798321000	-0.246105000
C	-1.168865000	-2.357554000	-1.002653000
H	-1.432918000	-3.365434000	-1.364273000
H	-0.994494000	-1.748058000	-1.900546000
C	-3.549935000	0.191511000	0.528815000
C	-4.663843000	-0.647574000	0.599491000
H	-5.602685000	-0.175446000	0.876697000
C	-4.684637000	-2.022399000	0.338088000
C	-3.496534000	-2.573159000	-0.136164000
H	-3.452022000	-3.607873000	-0.463240000
C	-3.731902000	1.730762000	0.785083000
C	-5.998060000	-2.837002000	0.588548000
O	2.865392000	-1.127357000	-0.236374000
C	3.343927000	-2.364260000	-0.380116000
C	2.475102000	-3.378536000	-0.841561000
C	1.102972000	-3.022294000	-1.333699000
H	1.176832000	-2.272255000	-2.135569000
H	0.646926000	-3.918808000	-1.784837000
C	4.700293000	-2.718833000	-0.101336000
C	5.055108000	-4.065880000	-0.198857000
H	6.074092000	-4.339359000	0.033599000
C	4.185846000	-5.095363000	-0.592818000
C	2.893146000	-4.709850000	-0.931250000
H	2.171078000	-5.436931000	-1.288285000
C	-6.231663000	-2.890962000	2.125185000
H	-5.356755000	-3.313645000	2.609591000
H	-6.399208000	-1.900030000	2.533537000
H	-7.084480000	-3.515599000	2.370291000
C	2.818808000	5.539377000	0.275675000
H	2.262484000	5.948485000	1.132109000
H	3.708809000	5.061837000	0.702901000
Si	3.359554000	7.068444000	-0.733209000
C	4.470042000	6.634429000	-2.215395000
H	5.351055000	6.060278000	-1.904724000
H	3.929960000	6.048137000	-2.967092000
H	4.825478000	7.550667000	-2.702424000
C	4.334075000	8.207936000	0.436524000
H	5.234205000	7.711493000	0.818328000
H	4.651709000	9.122243000	-0.078616000
H	3.724914000	8.505201000	1.298267000
C	1.822850000	7.989106000	-1.365322000
H	1.237528000	7.372321000	-2.056983000

H	1. 165087000	8. 275766000	-0. 536422000
H	2. 109050000	8. 903742000	-1. 898066000
N	1. 135100000	1. 677110000	-1. 607609000
C	2. 210463000	2. 449747000	-2. 033084000
C	0. 516097000	0. 903883000	-2. 538491000
C	2. 815563000	2. 127873000	-3. 294904000
C	2. 718755000	3. 534099000	-1. 294618000
C	0. 985407000	0. 664633000	-3. 812965000
H	-0. 420386000	0. 456583000	-2. 201761000
C	2. 218563000	1. 258003000	-4. 170102000
H	3. 727754000	2. 649774000	-3. 572600000
C	1. 936721000	4. 491178000	-0. 435271000
H	0. 429198000	0. 035041000	-4. 499671000
H	2. 668184000	1. 058662000	-5. 139639000
H	1. 320030000	3. 949450000	0. 289812000
H	1. 225083000	5. 058323000	-1. 073545000
C	-5. 025951000	2. 206269000	0. 063283000
C	-5. 157439000	1. 969311000	-1. 308288000
C	-6. 046458000	2. 898255000	0. 702002000
C	-6. 265215000	2. 404246000	-2. 009202000
H	-4. 378454000	1. 429690000	-1. 830390000
C	-7. 163089000	3. 336665000	-0. 000150000
H	-5. 989158000	3. 108125000	1. 759460000
C	-7. 278425000	3. 093458000	-1. 354980000
H	-8. 147852000	3. 434930000	-1. 901363000
C	2. 339368000	2. 356842000	2. 508304000
C	2. 232148000	3. 019124000	3. 754671000
C	1. 098060000	2. 892840000	4. 530752000
C	0. 041453000	2. 109304000	4. 054992000
C	0. 206293000	1. 473161000	2. 836733000
N	1. 320377000	1. 552174000	2. 078099000
H	1. 024070000	3. 408607000	5. 484872000
H	3. 059730000	3. 641912000	4. 081475000
H	-0. 889293000	2. 003101000	4. 601548000
H	-0. 601136000	0. 876991000	2. 422223000
C	3. 525385000	2. 592761000	1. 723905000
H	4. 220284000	3. 291788000	2. 184094000
C	3. 815273000	2. 149793000	0. 469518000
H	4. 779945000	2. 379184000	0. 029731000
H	3. 298377000	1. 328357000	-0. 006715000
H	3. 614579000	3. 967483000	-1. 738901000
C	-5. 878970000	-4. 301201000	0. 077862000
H	-5. 661444000	-4. 332805000	-0. 984371000
H	-5. 096737000	-4. 834814000	0. 608089000

H	-6.816143000	-4.822954000	0.246506000
C	5.769510000	-1.624535000	0.243450000
C	4.702001000	-6.571463000	-0.658582000
C	5.817834000	-0.592217000	-0.916354000
H	4.837150000	-0.171107000	-1.098692000
H	6.505149000	0.213498000	-0.677550000
H	6.158661000	-1.071342000	-1.828800000
C	5.411940000	-0.920416000	1.580301000
H	4.448007000	-0.433208000	1.517089000
H	5.384335000	-1.640742000	2.392325000
H	6.156721000	-0.167793000	1.819918000
C	5.202118000	-7.011458000	0.746150000
H	5.557651000	-8.037071000	0.714772000
H	6.017042000	-6.382350000	1.087658000
H	4.398082000	-6.952438000	1.473530000
C	3.587724000	-7.553673000	-1.104586000
H	2.748255000	-7.533917000	-0.417248000
H	3.226754000	-7.312710000	-2.098995000
H	3.980390000	-8.565500000	-1.126264000
C	-7.179268000	-2.167588000	-0.166808000
C	-8.400539000	-1.882870000	0.430627000
C	-7.029491000	-1.868565000	-1.523161000
C	-9.437814000	-1.314852000	-0.298629000
H	-8.563037000	-2.098332000	1.476139000
C	-8.059349000	-1.304682000	-2.251751000
H	-6.086374000	-2.076151000	-2.011066000
C	-9.273751000	-1.024018000	-1.639732000
H	-10.379026000	-1.100688000	0.191768000
H	-7.916645000	-1.080534000	-3.301309000
H	-10.081779000	-0.580948000	-2.207130000
C	-3.808815000	1.952409000	2.322441000
H	-3.878044000	3.008258000	2.563707000
H	-4.663507000	1.440677000	2.752641000
H	-2.911920000	1.560236000	2.790192000
C	-2.568707000	2.600811000	0.227245000
H	-1.658508000	2.452469000	0.792827000
H	-2.366022000	2.371594000	-0.812525000
H	-2.844208000	3.649095000	0.297834000
H	-7.944617000	3.872605000	0.523486000
H	-6.342325000	2.206501000	-3.070842000
C	5.872903000	-6.670939000	-1.676141000
H	5.545301000	-6.363899000	-2.664691000
H	6.703662000	-6.038980000	-1.381291000
H	6.231550000	-7.694139000	-1.737901000

C	7.196539000	-2.215976000	0.401340000
H	7.250360000	-2.915772000	1.228723000
H	7.519370000	-2.720704000	-0.502943000
H	7.895309000	-1.409602000	0.601320000

TS2^d_{syn}, $E_{(\text{SCF Done})} = -2853.499288 \text{ a.u.}$ IF = $i197.31 \text{ cm}^{-1}$

Y	1.405482000	0.321204000	0.427877000
N	0.199548000	2.624579000	0.117887000
C	0.217842000	3.034770000	-1.299479000
H	1.137532000	3.600702000	-1.474995000
H	-0.626534000	3.703927000	-1.531259000
C	0.171174000	1.835695000	-2.235714000
H	-0.749268000	1.266317000	-2.106793000
H	0.232823000	2.167635000	-3.280318000
O	1.244956000	0.923319000	-1.965188000
C	2.438766000	1.176397000	-2.707900000
H	3.139253000	0.383198000	-2.445173000
H	2.871775000	2.149445000	-2.452215000
H	2.217938000	1.130292000	-3.781356000
O	-0.693250000	-0.186181000	0.200298000
C	-1.914107000	0.244150000	-0.096458000
C	-2.169470000	1.637922000	-0.030669000
C	-1.185132000	2.548651000	0.648147000
H	-1.607494000	3.568023000	0.651709000
H	-1.083372000	2.262841000	1.704123000
C	-2.991608000	-0.604053000	-0.485285000
C	-4.162404000	0.001768000	-0.957410000
H	-4.959640000	-0.650916000	-1.298548000
C	-4.386470000	1.382655000	-0.997763000
C	-3.368458000	2.185415000	-0.488431000
H	-3.488935000	3.262435000	-0.423842000
C	-2.937728000	-2.175716000	-0.501883000
C	-5.721239000	1.928589000	-1.608899000
O	2.992332000	1.788530000	0.458672000
C	3.265838000	3.080539000	0.303987000
C	2.259783000	4.043221000	0.531210000
C	0.911076000	3.597992000	1.001839000
H	0.990019000	3.110867000	1.985686000
H	0.274108000	4.486587000	1.142995000
C	4.547806000	3.539091000	-0.100144000
C	4.766721000	4.907154000	-0.258624000
H	5.756118000	5.235713000	-0.568516000
C	3.772841000	5.868664000	-0.036159000
C	2.519445000	5.405888000	0.357673000

H	1.716855000	6.118012000	0.541653000
C	-5.701720000	1.630243000	-3.134949000
H	-4.812371000	2.068274000	-3.577537000
H	-5.685696000	0.563139000	-3.328860000
H	-6.567557000	2.059069000	-3.628948000
C	6.545182000	-1.704439000	-0.480631000
H	7.207486000	-0.925641000	-0.890855000
H	7.077996000	-2.102194000	0.396627000
Si	6.469999000	-3.080767000	-1.803953000
C	5.943123000	-4.758883000	-1.090786000
H	6.592609000	-5.053702000	-0.257791000
H	4.911530000	-4.731262000	-0.725279000
H	6.009873000	-5.540249000	-1.857708000
C	8.226074000	-3.262828000	-2.516427000
H	8.945743000	-3.523930000	-1.731193000
H	8.264953000	-4.051098000	-3.277674000
H	8.565773000	-2.330331000	-2.982770000
C	5.283958000	-2.579490000	-3.200813000
H	4.261106000	-2.470637000	-2.823649000
H	5.585604000	-1.627390000	-3.654535000
H	5.271523000	-3.337372000	-3.993017000
N	2.332097000	-1.672308000	-0.574548000
C	3.120858000	-2.433717000	0.290562000
C	1.421260000	-2.326399000	-1.341620000
C	2.662510000	-3.751069000	0.628060000
C	4.337209000	-1.938289000	0.786063000
C	1.115142000	-3.661334000	-1.215969000
H	0.898004000	-1.699666000	-2.060218000
C	1.702691000	-4.363310000	-0.134082000
H	3.169947000	-4.284055000	1.427957000
C	5.231053000	-1.035357000	-0.024275000
H	0.391784000	-4.129027000	-1.873867000
H	1.410037000	-5.389583000	0.075559000
H	5.498800000	-0.135514000	0.544670000
H	4.673697000	-0.673676000	-0.896676000
C	-4.339405000	-2.752598000	-0.149620000
C	-4.944062000	-2.375311000	1.053656000
C	-5.007797000	-3.671963000	-0.947497000
C	-6.165084000	-2.892941000	1.438614000
H	-4.449329000	-1.656375000	1.692781000
C	-6.237063000	-4.195294000	-0.563402000
H	-4.581176000	-3.996922000	-1.884455000
C	-6.820793000	-3.810740000	0.627804000
H	-7.777869000	-4.217846000	0.926522000

C	1.869580000	-0.744341000	3.855231000
C	1.329776000	-1.110645000	5.118704000
C	0.001064000	-0.919627000	5.413115000
C	-0.831781000	-0.373449000	4.424619000
C	-0.264062000	-0.065522000	3.204436000
N	1.044045000	-0.219424000	2.888169000
H	-0.394173000	-1.194233000	6.388051000
H	2.004984000	-1.535400000	5.855895000
H	-1.893279000	-0.217487000	4.584923000
H	-0.896491000	0.286957000	2.399112000
C	3.268213000	-0.947499000	3.652456000
H	3.752849000	-1.540511000	4.425824000
C	4.034608000	-0.520146000	2.598627000
H	4.860639000	-2.645106000	1.429002000
C	-5.854660000	3.468099000	-1.432134000
H	-5.821545000	3.750476000	-0.385340000
H	-5.060207000	3.988929000	-1.956853000
H	-6.803396000	3.801118000	-1.842008000
C	5.684954000	2.545087000	-0.343471000
C	4.068155000	7.364617000	-0.209742000
H	5.112241000	-0.622023000	2.678192000
H	3.727054000	0.293871000	1.945974000
C	-6.928626000	1.264634000	-0.890678000
C	-7.990436000	0.679880000	-1.569043000
C	-6.977090000	1.284782000	0.505417000
C	-9.063823000	0.130004000	-0.879049000
H	-7.997474000	0.642284000	-2.648165000
C	-8.043605000	0.740276000	1.194784000
H	-6.160279000	1.730210000	1.057648000
C	-9.096755000	0.157711000	0.502287000
H	-9.877584000	-0.321830000	-1.432133000
H	-8.055995000	0.767815000	2.277027000
H	-9.932933000	-0.270897000	1.039156000
H	-6.735750000	-4.909529000	-1.206395000
H	-6.611523000	-2.580961000	2.374261000
C	-2.467147000	-2.612304000	-1.916864000
H	-2.342205000	-3.688568000	-1.976333000
H	-3.176019000	-2.301471000	-2.677553000
H	-1.511101000	-2.149548000	-2.136614000
C	-1.953818000	-2.761654000	0.552116000
H	-2.148077000	-2.351662000	1.536972000
H	-2.078260000	-3.839366000	0.601905000
H	-0.927546000	-2.551290000	0.285756000
H	4.778571000	7.709491000	0.538907000

H	3.159692000	7.949809000	-0.107970000
H	4.496817000	7.566029000	-1.188631000
H	6.550023000	3.052813000	-0.757935000
H	5.985734000	2.066330000	0.585056000
H	5.381521000	1.763318000	-1.033884000

TS2^D_{iso}, $E_{(\text{SCF Done})} = -2853.487101 \text{ a.u.}$ IF = $i206.14 \text{ cm}^{-1}$

Y	-1.267123000	0.894369000	0.175858000
N	0.266436000	2.894703000	-0.458804000
C	0.610284000	3.711965000	0.720192000
H	-0.131968000	4.511650000	0.808294000
H	1.596688000	4.187163000	0.600571000
C	0.606353000	2.872158000	1.985779000
H	1.341472000	2.067931000	1.924862000
H	0.827103000	3.487851000	2.867221000
O	-0.667005000	2.231209000	2.163325000
C	-1.641614000	3.012090000	2.855405000
H	-2.505969000	2.365387000	3.014845000
H	-1.945639000	3.888509000	2.272590000
H	-1.239663000	3.324129000	3.826714000
O	0.686679000	0.035230000	0.226649000
C	2.013573000	0.221064000	0.163058000
C	2.441202000	1.485041000	-0.312614000
C	1.489784000	2.338599000	-1.110258000
H	2.055810000	3.185654000	-1.532692000
H	1.120998000	1.759149000	-1.968677000
C	2.995194000	-0.743940000	0.560186000
C	4.313360000	-0.284841000	0.582846000
H	5.067867000	-1.007322000	0.882554000
C	4.749513000	1.003813000	0.252499000
C	3.779968000	1.870360000	-0.245346000
H	4.050779000	2.850864000	-0.625884000
C	2.694672000	-2.245683000	0.907345000
C	6.254471000	1.384791000	0.456455000
O	-2.672730000	2.416112000	-0.344716000
C	-2.757482000	3.729402000	-0.527152000
C	-1.660562000	4.446573000	-1.048073000
C	-0.433795000	3.706438000	-1.499568000
H	-0.697355000	3.003420000	-2.303465000
H	0.279396000	4.427393000	-1.932588000
C	-3.942060000	4.430896000	-0.193060000
C	-3.985593000	5.812853000	-0.367738000
H	-4.900130000	6.340024000	-0.105649000
C	-2.899769000	6.543080000	-0.871292000

C	-1.746468000	5.833834000	-1.205926000
H	-0.888871000	6.367586000	-1.611965000
C	6.525803000	1.426933000	1.987232000
H	5.833359000	2.117678000	2.458567000
H	6.389751000	0.450131000	2.438967000
H	7.534205000	1.768398000	2.197169000
C	-5.093046000	-3.631425000	0.341018000
H	-4.815306000	-4.193391000	1.245038000
H	-5.776604000	-2.843302000	0.681557000
Si	-6.069693000	-4.875809000	-0.731249000
C	-6.723023000	-4.124727000	-2.352181000
H	-7.354747000	-3.247860000	-2.166776000
H	-5.904252000	-3.821395000	-3.013824000
H	-7.330238000	-4.862221000	-2.891229000
C	-7.553794000	-5.473064000	0.297305000
H	-8.225388000	-4.641735000	0.542841000
H	-8.138099000	-6.221488000	-0.250960000
H	-7.227305000	-5.929217000	1.239358000
C	-4.958138000	-6.357848000	-1.149532000
H	-4.097883000	-6.058004000	-1.758884000
H	-4.573469000	-6.833402000	-0.239800000
H	-5.515112000	-7.115317000	-1.713653000
N	-1.924182000	-0.827143000	-1.531379000
C	-3.213814000	-1.114760000	-1.963707000
C	-1.025887000	-0.420404000	-2.469003000
C	-3.614513000	-0.644466000	-3.260401000
C	-4.131344000	-1.861275000	-1.201668000
C	-1.337288000	-0.082003000	-3.769090000
H	0.002254000	-0.363797000	-2.111351000
C	-2.698910000	-0.142383000	-4.148096000
H	-4.655343000	-0.765155000	-3.549655000
C	-3.823405000	-3.004797000	-0.271598000
H	-0.561568000	0.230298000	-4.460589000
H	-3.010521000	0.168749000	-5.142146000
H	-3.132885000	-2.691644000	0.520197000
H	-3.296837000	-3.811330000	-0.824949000
C	3.795607000	-3.140876000	0.268892000
C	4.018932000	-3.054365000	-1.108619000
C	4.543796000	-4.062134000	0.989766000
C	4.953717000	-3.854211000	-1.736249000
H	3.452460000	-2.342533000	-1.694220000
C	5.485876000	-4.868284000	0.361421000
H	4.405444000	-4.168051000	2.055212000
C	5.695315000	-4.769714000	-1.000318000

H	6.428767000	-5.397437000	-1.489253000
C	-3.405978000	-0.777418000	2.535581000
C	-3.556703000	-1.390851000	3.803334000
C	-2.461231000	-1.659857000	4.597735000
C	-1.186605000	-1.330599000	4.122902000
C	-1.098087000	-0.719869000	2.884478000
N	-2.158392000	-0.416446000	2.105073000
H	-2.588776000	-2.134231000	5.567555000
H	-4.556886000	-1.657629000	4.132049000
H	-0.286171000	-1.550478000	4.686057000
H	-0.124590000	-0.468838000	2.472150000
C	-4.590775000	-0.594836000	1.734626000
H	-5.486912000	-1.008978000	2.191775000
C	-4.704508000	-0.100661000	0.469050000
H	-5.691441000	-0.008437000	0.026166000
H	-3.949656000	0.505113000	-0.014275000
H	-5.116494000	-1.919889000	-1.662525000
C	6.579878000	2.792610000	-0.118821000
H	6.362639000	2.845878000	-1.180234000
H	6.008680000	3.561679000	0.391138000
H	7.634802000	3.008170000	0.021279000
C	-5.143189000	3.649421000	0.345961000
C	-2.995829000	8.063372000	-1.060505000
C	7.156879000	0.354222000	-0.276821000
C	8.243324000	-0.268964000	0.323823000
C	6.894371000	0.061599000	-1.617361000
C	9.040169000	-1.157980000	-0.386905000
H	8.485759000	-0.072313000	1.357500000
C	7.685470000	-0.821093000	-2.327567000
H	6.051033000	0.530077000	-2.107175000
C	8.766953000	-1.437682000	-1.712487000
H	9.879689000	-1.632077000	0.105718000
H	7.459126000	-1.032222000	-3.365054000
H	9.387561000	-2.130696000	-2.265424000
C	2.663477000	-2.377394000	2.456631000
H	2.401573000	-3.386035000	2.759843000
H	3.623200000	-2.120844000	2.893312000
H	1.918162000	-1.701304000	2.862474000
C	1.333592000	-2.753802000	0.349356000
H	0.500076000	-2.298747000	0.867559000
H	1.235678000	-2.540224000	-0.708769000
H	1.272069000	-3.829446000	0.486851000
H	6.056195000	-5.577145000	0.948326000
H	5.107571000	-3.765902000	-2.804263000

H	-2.037524000	8.474406000	-1.361727000
H	-3.727321000	8.313517000	-1.826205000
H	-3.302922000	8.552010000	-0.138775000
H	-5.974585000	4.316844000	0.549500000
H	-5.469710000	2.901871000	-0.372935000
H	-4.889815000	3.127766000	1.266988000

TS2^E_{syn}, $E_{(\text{SCF Done})} = -3752.375207 \text{ a.u.}$ IF = $i239.27 \text{ cm}^{-1}$

Y	1.540694000	0.159799000	0.373661000
N	1.565926000	2.715868000	0.203006000
C	1.653386000	3.149861000	-1.203837000
H	2.707753000	3.155329000	-1.491832000
H	1.273933000	4.177036000	-1.327900000
C	0.881573000	2.218902000	-2.123740000
H	-0.178756000	2.214120000	-1.880491000
H	0.998700000	2.534218000	-3.168045000
O	1.342183000	0.865105000	-1.984133000
C	2.299464000	0.474534000	-2.967328000
H	2.570531000	-0.559097000	-2.751223000
H	3.194318000	1.102833000	-2.919729000
H	1.846174000	0.535587000	-3.964288000
O	-0.592298000	0.713528000	0.350882000
C	-1.448154000	1.723805000	0.227762000
C	-0.974071000	3.051927000	0.381145000
C	0.409641000	3.327376000	0.895545000
H	0.559360000	4.420390000	0.904041000
H	0.489480000	3.011010000	1.943268000
C	-2.846130000	1.562142000	-0.053677000
C	-3.626303000	2.710372000	-0.209903000
H	-4.679921000	2.574425000	-0.400291000
C	-3.149457000	4.024419000	-0.126193000
C	-1.801604000	4.159773000	0.184102000
H	-1.356609000	5.142297000	0.305320000
C	-3.512011000	0.127515000	-0.110863000
C	-4.124333000	5.227590000	-0.349395000
C	-5.254169000	5.189438000	0.717583000
H	-5.933402000	6.024960000	0.576390000
H	-4.836346000	5.255179000	1.717579000
H	-5.828127000	4.271628000	0.647898000
O	3.693955000	0.685418000	0.047358000
C	4.516970000	1.726589000	-0.113899000
C	4.077092000	2.996104000	0.326286000
C	2.759831000	3.109972000	1.016780000
H	2.733523000	2.485276000	1.922797000

H	2.629294000	4.150210000	1.353240000
C	5.826324000	1.672923000	-0.706304000
C	6.526873000	2.871618000	-0.864149000
H	7.504067000	2.824366000	-1.320530000
C	6.072118000	4.136363000	-0.465454000
C	4.827939000	4.161121000	0.149647000
H	4.401228000	5.090550000	0.512127000
C	-4.753338000	5.132331000	-1.767819000
H	-3.980673000	5.157066000	-2.530273000
H	-5.318437000	4.213972000	-1.885182000
H	-5.426293000	5.967526000	-1.937825000
C	5.122448000	-4.309133000	-0.017279000
H	6.055592000	-4.045531000	-0.539188000
H	5.427696000	-4.557258000	1.011108000
Si	4.488482000	-5.902072000	-0.861765000
C	3.240848000	-6.857776000	0.203276000
H	3.641521000	-7.054774000	1.204799000
H	2.306938000	-6.297069000	0.312974000
H	3.002150000	-7.824661000	-0.256405000
C	5.998095000	-7.022841000	-1.159388000
H	6.499061000	-7.273652000	-0.216517000
H	5.701475000	-7.963782000	-1.637928000
H	6.735172000	-6.535748000	-1.808749000
C	3.691032000	-5.471088000	-2.530986000
H	2.792470000	-4.859951000	-2.388136000
H	4.384077000	-4.911164000	-3.170428000
H	3.396070000	-6.378300000	-3.071541000
N	1.403559000	-2.097139000	-0.508124000
C	1.714452000	-3.084487000	0.434472000
C	0.351832000	-2.336191000	-1.336516000
C	0.695502000	-4.034211000	0.777376000
C	3.021267000	-3.220414000	0.924597000
C	-0.493751000	-3.413405000	-1.222694000
H	0.185408000	-1.583967000	-2.103586000
C	-0.355636000	-4.235677000	-0.075540000
H	0.860183000	-4.682157000	1.634161000
C	4.203243000	-3.070688000	-0.003034000
H	-1.290913000	-3.566586000	-1.938316000
H	-1.068885000	-5.034802000	0.112997000
H	4.821028000	-2.202957000	0.247540000
H	3.830308000	-2.871852000	-1.015745000
C	-3.080016000	-0.628329000	1.183409000
C	-2.634084000	-1.944619000	1.207979000
C	-3.202203000	0.017019000	2.414526000

C	-2.359609000	-2.588721000	2.404529000
H	-2.500663000	-2.490223000	0.287663000
C	-2.939498000	-0.631165000	3.608952000
H	-3.537084000	1.045215000	2.443591000
C	-2.521269000	-1.958132000	3.634759000
C	-3.140755000	-0.619109000	-1.430375000
C	-3.766786000	-1.833281000	-1.745018000
C	-2.330686000	-0.066557000	-2.406299000
C	-3.571851000	-2.451665000	-2.959726000
H	-4.443509000	-2.284830000	-1.032170000
C	-2.129666000	-0.693807000	-3.634147000
H	-1.867055000	0.892514000	-2.237823000
C	-2.742870000	-1.895853000	-3.942092000
C	-5.080592000	0.232566000	-0.154045000
C	-5.914340000	-0.101820000	0.906042000
C	-5.708123000	0.645555000	-1.331814000
C	-7.293989000	-0.015276000	0.797856000
H	-5.498773000	-0.447336000	1.839822000
C	-7.083374000	0.735859000	-1.438929000
H	-5.106001000	0.904204000	-2.192080000
C	-7.915555000	0.407186000	-0.371603000
C	2.119822000	-0.433481000	3.935717000
C	1.818190000	-0.150237000	5.292807000
C	0.767240000	0.669149000	5.636393000
C	-0.041311000	1.177915000	4.611771000
C	0.283857000	0.851869000	3.308144000
N	1.353674000	0.110677000	2.933290000
H	0.560832000	0.896431000	6.679209000
H	2.451969000	-0.589613000	6.057467000
H	-0.914248000	1.789070000	4.813869000
H	-0.364212000	1.165686000	2.499279000
C	3.210213000	-1.322737000	3.671089000
H	3.541831000	-1.898506000	4.533261000
C	3.822219000	-1.543487000	2.473177000
H	3.123989000	-3.988982000	1.689483000
C	-3.393536000	6.590691000	-0.234539000
H	-2.966322000	6.725712000	0.753659000
H	-2.599215000	6.673251000	-0.969234000
H	-4.097642000	7.398401000	-0.408659000
C	6.533659000	0.320986000	-1.067586000
C	6.958362000	5.402763000	-0.706332000
H	4.692966000	-2.189100000	2.445915000
H	3.766756000	-0.839367000	1.649440000
C	6.849819000	-0.414213000	0.263711000

H	5.955864000	-0.523886000	0.864262000
H	7.263986000	-1.399339000	0.071958000
H	7.574579000	0.154561000	0.838434000
C	7.877426000	0.514908000	-1.822772000
H	8.615064000	1.024382000	-1.212695000
H	8.279473000	-0.459919000	-2.081141000
H	7.739675000	1.074133000	-2.742440000
C	5.625725000	-0.540877000	-1.980376000
H	4.658162000	-0.686082000	-1.523789000
H	5.490473000	-0.050798000	-2.939380000
H	6.077271000	-1.511562000	-2.157218000
C	7.234436000	5.564744000	-2.227634000
H	7.844055000	6.445141000	-2.408290000
H	7.760012000	4.703051000	-2.624854000
H	6.303221000	5.677629000	-2.774509000
C	8.308908000	5.247547000	0.047569000
H	8.928296000	6.126566000	-0.104533000
H	8.138781000	5.130426000	1.113489000
H	8.858317000	4.381926000	-0.306462000
C	6.266337000	6.694929000	-0.199694000
H	5.323170000	6.861009000	-0.709922000
H	6.078333000	6.646650000	0.867830000
H	6.906332000	7.551016000	-0.389584000
H	-7.500249000	1.066078000	-2.378427000
H	-7.890465000	-0.291516000	1.656233000
H	-1.493043000	-0.201897000	-4.353985000
H	-4.087153000	-3.381982000	-3.154351000
H	-3.080072000	-0.082633000	4.527929000
H	-2.027970000	-3.616525000	2.365491000
C	-9.463792000	0.487224000	-0.444027000
C	-9.963164000	0.981343000	-1.826685000
H	-9.589083000	1.975586000	-2.047652000
H	-9.652481000	0.309590000	-2.620056000
H	-11.047846000	1.022619000	-1.826841000
C	-9.982702000	1.474902000	0.638937000
H	-11.065320000	1.545320000	0.594039000
H	-9.706189000	1.146179000	1.634898000
H	-9.569663000	2.466430000	0.479921000
C	-10.067914000	-0.922137000	-0.186665000
H	-9.714218000	-1.629827000	-0.930336000
H	-9.793640000	-1.293500000	0.794828000
H	-11.151544000	-0.881327000	-0.242716000
C	-2.575610000	-2.613597000	-5.308141000
C	-1.605386000	-1.858451000	-6.253516000

H	-1.970931000	-0.862241000	-6.479710000
H	-0.616413000	-1.774563000	-5.814989000
H	-1.513413000	-2.402329000	-7.188367000
C	-2.012964000	-4.045536000	-5.084784000
H	-2.678325000	-4.637651000	-4.466004000
H	-1.896244000	-4.553298000	-6.037404000
H	-1.042525000	-4.003445000	-4.599796000
C	-3.959719000	-2.709600000	-6.010503000
H	-4.663833000	-3.278355000	-5.412754000
H	-4.373689000	-1.719322000	-6.174837000
H	-3.858250000	-3.201132000	-6.973393000
C	-2.259242000	-2.744603000	4.946978000
C	-2.475121000	-1.871081000	6.210222000
H	-2.276257000	-2.462104000	7.098727000
H	-1.805294000	-1.017892000	6.217179000
H	-3.496517000	-1.509927000	6.269322000
C	-0.796221000	-3.269368000	4.964192000
H	-0.606321000	-3.931230000	4.126523000
H	-0.093992000	-2.443535000	4.911024000
H	-0.606703000	-3.819811000	5.880828000
C	-3.236511000	-3.952001000	5.023381000
H	-4.267039000	-3.610143000	5.010165000
H	-3.090499000	-4.626965000	4.186947000
H	-3.073663000	-4.509236000	5.941035000

TS2^B_{iso}, $E_{\text{(SCF Done)}} = -3752.379405$ a.u. IF = $i143.10$ cm⁻¹

Y	1.695065000	-0.321056000	-0.113777000
N	1.757107000	-2.684189000	-1.049878000
C	1.687979000	-3.700677000	0.018951000
H	2.711900000	-3.969193000	0.295158000
H	1.187114000	-4.614687000	-0.335069000
C	0.953182000	-3.172563000	1.240490000
H	-0.081126000	-2.929138000	1.003612000
H	0.966323000	-3.912467000	2.050536000
O	1.551327000	-1.950675000	1.709616000
C	2.578580000	-2.127130000	2.685022000
H	2.868970000	-1.131671000	3.021623000
H	3.450488000	-2.637066000	2.261496000
H	2.181609000	-2.694561000	3.534885000
O	-0.400506000	-0.772759000	-0.424987000
C	-1.296381000	-1.693072000	-0.828890000
C	-0.773582000	-2.825552000	-1.495806000
C	0.632096000	-2.813986000	-2.016480000
H	0.795282000	-3.738291000	-2.594460000

H	0.761510000	-1.987274000	-2.730160000
C	-2.721646000	-1.617270000	-0.609682000
C	-3.451944000	-2.721424000	-1.050340000
H	-4.524112000	-2.660832000	-0.932567000
C	-2.945016000	-3.896197000	-1.619726000
C	-1.577216000	-3.907045000	-1.858381000
H	-1.105296000	-4.742218000	-2.366855000
C	-3.421998000	-0.326145000	-0.039889000
C	-3.908249000	-5.073685000	-1.983304000
C	-4.950320000	-4.595782000	-3.033011000
H	-5.618248000	-5.410280000	-3.297238000
H	-4.452770000	-4.256019000	-3.936253000
H	-5.549840000	-3.778649000	-2.646380000
O	3.844451000	-0.743324000	-0.183440000
C	4.687840000	-1.771127000	-0.307925000
C	4.283700000	-2.880690000	-1.082341000
C	3.006092000	-2.805974000	-1.857301000
H	3.020056000	-1.935003000	-2.530062000
H	2.927882000	-3.697589000	-2.500477000
C	5.991266000	-1.819661000	0.283776000
C	6.723252000	-3.002220000	0.155650000
H	7.694947000	-3.047525000	0.625035000
C	6.300564000	-4.136292000	-0.554604000
C	5.068927000	-4.032083000	-1.190371000
H	4.683712000	-4.844845000	-1.797506000
C	-4.649406000	-5.551671000	-0.703075000
H	-3.939346000	-5.891860000	0.044658000
H	-5.241753000	-4.751986000	-0.271631000
H	-5.315468000	-6.376012000	-0.939893000
C	2.136486000	5.532343000	0.845477000
H	1.328993000	5.806241000	1.541023000
H	2.937452000	5.125603000	1.473663000
Si	2.745190000	7.199525000	0.133838000
C	4.424000000	7.081007000	-0.755684000
H	5.169460000	6.563111000	-0.140767000
H	4.347402000	6.552234000	-1.712235000
H	4.808520000	8.086535000	-0.966045000
C	2.953583000	8.369687000	1.619000000
H	3.687612000	7.977519000	2.333211000
H	3.298177000	9.359709000	1.297872000
H	2.006043000	8.503179000	2.154138000
C	1.467603000	7.931634000	-1.064663000
H	1.341317000	7.302021000	-1.952807000
H	0.486543000	8.038736000	-0.587570000

H	1.783348000	8.925182000	-1.404535000
N	1.591787000	1.682746000	-1.679818000
C	2.474186000	2.738113000	-1.882051000
C	1.283798000	0.913137000	-2.756072000
C	3.249466000	2.747809000	-3.088711000
C	2.652498000	3.795029000	-0.962320000
C	1.919716000	0.962518000	-3.980345000
H	0.460523000	0.216674000	-2.591551000
C	2.982936000	1.881788000	-4.118676000
H	4.017166000	3.509723000	-3.195870000
C	1.599302000	4.444076000	-0.103502000
H	1.612421000	0.309811000	-4.790702000
H	3.557151000	1.931092000	-5.040485000
H	1.039899000	3.690306000	0.461016000
H	0.851799000	4.946074000	-0.751878000
C	-2.822196000	0.916345000	-0.768320000
C	-2.565162000	2.135910000	-0.162093000
C	-2.643292000	0.852378000	-2.156412000
C	-2.224509000	3.260757000	-0.909971000
H	-2.653555000	2.245760000	0.907876000
C	-2.300677000	1.964391000	-2.893618000
H	-2.818160000	-0.082197000	-2.671564000
C	-2.119551000	3.213331000	-2.291615000
C	-3.302308000	-0.284896000	1.518015000
C	-4.013046000	0.662052000	2.257142000
C	-2.642196000	-1.271335000	2.242504000
C	-4.059078000	0.624800000	3.639888000
H	-4.582180000	1.424552000	1.743267000
C	-2.692896000	-1.313089000	3.627098000
H	-2.109644000	-2.052363000	1.721136000
C	-3.406847000	-0.371813000	4.362632000
C	-4.970481000	-0.375954000	-0.321011000
C	-5.601974000	0.373914000	-1.306816000
C	-5.790359000	-1.197467000	0.455139000
C	-6.971550000	0.301220000	-1.506221000
H	-5.031288000	1.038591000	-1.936569000
C	-7.156662000	-1.272941000	0.253971000
H	-5.353495000	-1.798089000	1.240838000
C	-7.785206000	-0.522464000	-0.735661000
C	2.172437000	2.140005000	2.494205000
C	1.745028000	2.629851000	3.749545000
C	0.499055000	2.303660000	4.245910000
C	-0.338814000	1.489651000	3.479720000
C	0.153542000	0.988835000	2.285369000

N	1. 385841000	1. 256074000	1. 804538000
H	0. 168568000	2. 699146000	5. 203095000
H	2. 402611000	3. 300402000	4. 294896000
H	-1. 346960000	1. 246080000	3. 788015000
H	-0. 474687000	0. 355408000	1. 660320000
C	3. 393032000	2. 669855000	1. 944604000
H	3. 886625000	3. 396605000	2. 586430000
C	3. 878262000	2. 496190000	0. 682404000
H	4. 815243000	2. 966208000	0. 403851000
H	3. 598046000	1. 657203000	0. 063319000
H	3. 454783000	4. 470340000	-1. 257119000
C	-3. 138812000	-6. 282235000	-2. 577051000
H	-2. 637061000	-6. 013574000	-3. 500780000
H	-2. 399103000	-6. 658494000	-1. 877859000
H	-3. 834782000	-7. 086222000	-2. 795327000
C	6. 622584000	-0. 564025000	0. 977888000
C	7. 213714000	-5. 405406000	-0. 618798000
C	6. 695666000	0. 579883000	-0. 070035000
H	5. 721109000	0. 766230000	-0. 503292000
H	7. 055789000	1. 495253000	0. 389226000
H	7. 377860000	0. 308790000	-0. 869802000
C	5. 774046000	-0. 132006000	2. 202981000
H	4. 764098000	0. 115906000	1. 906894000
H	5. 736982000	-0. 931374000	2. 936813000
H	6. 212538000	0. 741488000	2. 675196000
C	8. 066125000	-0. 821883000	1. 488845000
H	8. 731176000	-1. 104652000	0. 680017000
H	8. 452149000	0. 089881000	1. 934068000
H	8. 089423000	-1. 598211000	2. 246522000
C	8. 569748000	-5. 041317000	-1. 285819000
H	9. 094455000	-4. 280582000	-0. 717985000
H	9. 207110000	-5. 918588000	-1. 345540000
H	8. 410417000	-4. 666116000	-2. 292129000
C	7. 473529000	-5. 933216000	0. 820263000
H	8. 102063000	-6. 818230000	0. 788870000
H	7. 972753000	-5. 186358000	1. 428134000
H	6. 538362000	-6. 197374000	1. 304742000
C	6. 559611000	-6. 545804000	-1. 441534000
H	5. 612067000	-6. 849111000	-1. 008294000
H	6. 388709000	-6. 240686000	-2. 468623000
H	7. 215869000	-7. 410481000	-1. 453097000
C	-9. 314269000	-0. 569215000	-0. 997174000
C	-10. 045232000	-1. 544979000	-0. 038608000
H	-9. 679033000	-2. 559601000	-0. 155747000

H	-9.918286000	-1.247762000	0.997149000
H	-11.107703000	-1.543469000	-0.260813000
C	-9.575833000	-1.037637000	-2.456520000
H	-10.643341000	-1.081508000	-2.650221000
H	-9.129667000	-0.356733000	-3.173284000
H	-9.158642000	-2.026689000	-2.620024000
C	-9.917616000	0.849603000	-0.796223000
H	-9.477969000	1.564072000	-1.483751000
H	-10.989427000	0.828791000	-0.968914000
H	-9.742014000	1.198412000	0.216931000
C	-3.487393000	-0.489931000	5.908913000
C	-4.267988000	0.687899000	6.548514000
H	-3.801769000	1.640126000	6.317243000
H	-5.296204000	0.712550000	6.203551000
H	-4.279216000	0.571588000	7.627636000
C	-4.215969000	-1.813475000	6.277920000
H	-3.677865000	-2.675039000	5.896991000
H	-4.293739000	-1.911235000	7.356570000
H	-5.218382000	-1.825533000	5.860847000
C	-2.058138000	-0.507378000	6.520363000
H	-1.475412000	-1.339036000	6.139889000
H	-1.530922000	0.412962000	6.289961000
H	-2.116891000	-0.603107000	7.600260000
C	-1.844707000	4.459708000	-3.175059000
C	-1.845594000	5.773093000	-2.351004000
H	-1.680060000	6.616893000	-3.013316000
H	-2.797510000	5.918703000	-1.850548000
H	-1.058990000	5.773249000	-1.605637000
C	-2.958364000	4.582742000	-4.254798000
H	-2.795846000	5.471892000	-4.856277000
H	-2.964615000	3.725532000	-4.918672000
H	-3.936123000	4.661313000	-3.789060000
C	-0.466725000	4.310392000	-3.876904000
H	0.328966000	4.230176000	-3.143347000
H	-0.443688000	3.423982000	-4.501943000
H	-0.270196000	5.174502000	-4.504493000
H	-7.728611000	-1.931637000	0.889933000
H	-7.405617000	0.910932000	-2.286439000
H	-2.178382000	-2.117105000	4.134731000
H	-4.638276000	1.380290000	4.149231000
H	-2.068111000	4.188668000	-0.380311000
H	-2.200900000	1.862246000	-3.965135000

TS2⁶_{syn}, $E_{\text{(SCF Done)}} = -3477.350595$ a.u. IF = $i165.82$ cm⁻¹

Y	-1.141795000	0.072726000	0.404477000
N	-1.148602000	-2.489568000	0.198658000
C	-1.253859000	-2.890695000	-1.217987000
H	-2.314398000	-2.948367000	-1.475150000
H	-0.825592000	-3.893029000	-1.380296000
C	-0.555625000	-1.909194000	-2.152706000
H	0.514858000	-1.872407000	-1.962224000
H	-0.711667000	-2.216097000	-3.195013000
O	-1.040172000	-0.566003000	-1.983692000
C	-2.131228000	-0.242021000	-2.847012000
H	-2.419480000	0.787374000	-2.630260000
H	-2.985781000	-0.900222000	-2.668336000
H	-1.804072000	-0.316264000	-3.890773000
O	0.994079000	-0.443947000	0.291362000
C	1.836709000	-1.443515000	0.042374000
C	1.385140000	-2.777178000	0.209419000
C	0.055031000	-3.056903000	0.847116000
H	-0.069907000	-4.151134000	0.913494000
H	0.045200000	-2.689377000	1.881706000
C	3.192951000	-1.264883000	-0.385279000
C	3.954716000	-2.405553000	-0.659650000
H	4.985890000	-2.256838000	-0.944819000
C	3.488755000	-3.722643000	-0.574409000
C	2.184595000	-3.874439000	-0.115195000
H	1.758081000	-4.862176000	0.026665000
C	3.904369000	0.143646000	-0.295494000
C	4.431863000	-4.914256000	-0.946812000
C	5.671986000	-4.913134000	-0.009544000
H	6.327895000	-5.743813000	-0.252669000
H	5.366011000	-5.012545000	1.027480000
H	6.239287000	-3.994192000	-0.111172000
O	-3.210684000	-0.494159000	-0.009621000
C	-4.038080000	-1.532249000	-0.128103000
C	-3.652524000	-2.789141000	0.388054000
C	-2.309304000	-2.938157000	1.030064000
H	-2.250815000	-2.364914000	1.967923000
H	-2.166044000	-3.995516000	1.304536000
C	-5.297913000	-1.456900000	-0.780907000
C	-6.109266000	-2.592827000	-0.828527000
H	-7.072633000	-2.493549000	-1.316873000
C	-5.752981000	-3.834860000	-0.288333000
C	-4.492635000	-3.901603000	0.305238000
H	-4.127250000	-4.833530000	0.723910000
C	4.901566000	-4.764338000	-2.421075000

H	4.050031000	-4.765566000	-3.094770000
H	5.449148000	-3.839256000	-2.565754000
H	5.552832000	-5.589279000	-2.694230000
C	-4.976878000	4.001979000	-0.605660000
H	-5.681585000	3.603475000	-1.352591000
H	-5.608986000	4.433576000	0.185450000
Si	-4.040001000	5.426992000	-1.465588000
C	-3.222164000	6.620158000	-0.236813000
H	-3.960754000	7.016747000	0.470377000
H	-2.432445000	6.127787000	0.340026000
H	-2.776975000	7.471967000	-0.765589000
C	-5.316892000	6.412142000	-2.478173000
H	-6.102647000	6.819865000	-1.830842000
H	-4.843502000	7.254847000	-2.996175000
H	-5.801799000	5.784321000	-3.235216000
C	-2.730469000	4.717727000	-2.645814000
H	-1.978075000	4.144764000	-2.092067000
H	-3.188883000	4.053673000	-3.389163000
H	-2.214842000	5.519891000	-3.186808000
N	-1.132697000	2.515060000	0.330951000
C	-1.938637000	3.288904000	1.176154000
C	0.151915000	2.923584000	0.155857000
C	-1.288416000	4.201471000	2.076792000
C	-3.329919000	3.209291000	1.166980000
C	0.755251000	3.952630000	0.841300000
H	0.725067000	2.346986000	-0.563458000
C	0.017985000	4.556756000	1.888706000
H	-1.895016000	4.677817000	2.842202000
C	-4.156507000	2.830027000	-0.024161000
H	1.776466000	4.238578000	0.623520000
H	0.480224000	5.307368000	2.525775000
H	-4.858319000	2.028152000	0.238233000
H	-3.504571000	2.411496000	-0.800720000
C	3.953928000	0.426524000	1.239893000
C	3.262874000	1.444846000	1.868765000
C	4.698095000	-0.454918000	2.040377000
C	3.330429000	1.620156000	3.257555000
H	2.657631000	2.128096000	1.295065000
C	4.779897000	-0.303866000	3.408700000
H	5.225384000	-1.272892000	1.570847000
C	4.091605000	0.751863000	4.012491000
H	4.152947000	0.882625000	5.084673000
C	3.215247000	1.246832000	-1.153639000
C	3.633682000	2.573837000	-1.035367000

C	2.350756000	0.923825000	-2.193811000
C	3.181338000	3.558239000	-1.900633000
H	4.347733000	2.838391000	-0.268714000
C	1.885190000	1.894648000	-3.079078000
H	2.063832000	-0.105425000	-2.347696000
C	2.300166000	3.207904000	-2.919250000
H	1.948716000	3.967136000	-3.605445000
C	5.346647000	0.126227000	-0.913540000
C	6.457881000	0.606348000	-0.244299000
C	5.509445000	-0.273568000	-2.248098000
C	7.714416000	0.660084000	-0.856712000
H	6.370000000	0.956989000	0.772644000
C	6.738708000	-0.232960000	-2.875035000
H	4.649272000	-0.621256000	-2.802147000
C	7.846497000	0.234096000	-2.162777000
H	8.813471000	0.270506000	-2.646687000
C	5.610297000	-1.262360000	4.260040000
H	6.442538000	-0.740265000	4.727266000
H	5.007588000	-1.697085000	5.053806000
H	6.011957000	-2.068727000	3.655189000
C	2.573336000	2.771906000	3.915465000
H	1.518137000	2.739558000	3.656815000
H	2.665255000	2.726645000	4.995725000
H	2.964385000	3.729790000	3.580179000
C	3.654040000	5.004286000	-1.762599000
H	4.164820000	5.329312000	-2.666060000
H	2.810188000	5.671065000	-1.601322000
H	4.338142000	5.110100000	-0.927102000
C	0.950121000	1.523664000	-4.228483000
H	-0.033656000	1.963965000	-4.082419000
H	1.338748000	1.891644000	-5.174852000
H	0.835647000	0.447314000	-4.301447000
C	8.913649000	1.190389000	-0.073004000
H	9.806669000	1.196659000	-0.689322000
H	8.729475000	2.204630000	0.273338000
H	9.106332000	0.573079000	0.801539000
C	6.899047000	-0.683839000	-4.325580000
H	7.581248000	-1.528347000	-4.393726000
H	5.944405000	-0.982123000	-4.746271000
H	7.306029000	0.119001000	-4.935751000
C	-1.843031000	0.531274000	3.956714000
C	-1.428293000	0.386604000	5.308132000
C	-0.227998000	-0.199094000	5.636677000
C	0.610521000	-0.632635000	4.600829000

C	0.167952000	-0.460249000	3.303066000
N	-1.027101000	0.070851000	2.948239000
H	0.066298000	-0.306887000	6.677693000
H	-2.094181000	0.751376000	6.084628000
H	1.587395000	-1.065616000	4.786697000
H	0.819134000	-0.728826000	2.477803000
C	-3.104807000	1.173633000	3.732777000
H	-3.524984000	1.630611000	4.627003000
C	-3.794981000	1.321041000	2.561941000
H	-3.815336000	3.891257000	1.864392000
C	3.716043000	-6.282569000	-0.803227000
H	3.401964000	-6.456435000	0.220678000
H	2.844315000	-6.338902000	-1.447021000
H	4.394823000	-7.081190000	-1.085931000
C	-5.789904000	-0.137569000	-1.419256000
C	-6.738891000	-5.046340000	-0.382357000
H	-4.793145000	1.746301000	2.600505000
H	-3.601178000	0.718441000	1.681248000
C	-7.013325000	0.430542000	-0.658244000
H	-6.784547000	0.558529000	0.395140000
H	-7.299359000	1.395703000	-1.065713000
H	-7.864314000	-0.238466000	-0.741572000
C	-6.124678000	-0.302078000	-2.923005000
H	-6.970014000	-0.966924000	-3.067933000
H	-6.376870000	0.661446000	-3.356361000
H	-5.278971000	-0.707977000	-3.469133000
C	-7.035339000	-5.364252000	-1.874923000
H	-7.715070000	-6.207640000	-1.952380000
H	-7.491887000	-4.515856000	-2.373269000
H	-6.119341000	-5.615971000	-2.400826000
C	-8.067674000	-4.690398000	0.341502000
H	-8.759508000	-5.525957000	0.290590000
H	-7.882917000	-4.463585000	1.387097000
H	-8.543721000	-3.829077000	-0.114565000
C	-6.153801000	-6.321577000	0.278296000
H	-5.237019000	-6.632949000	-0.211544000
H	-5.945830000	-6.157958000	1.330602000
H	-6.869054000	-7.134389000	0.199341000
H	-4.977240000	0.578276000	-1.337508000

TS2⁶_{iso}, $E_{\text{(SCF Done)}} = -3477.349355 \text{ a.u.}$ IF = $i226.44 \text{ cm}^{-1}$

Y	1.243653000	-0.206974000	0.039844000
N	1.337135000	-2.652515000	-0.732214000
C	1.279264000	-3.584626000	0.410450000

H	2.306416000	-3.816647000	0.708113000
H	0.795920000	-4.532252000	0.125451000
C	0.530061000	-2.979467000	1.586505000
H	-0.503895000	-2.762207000	1.322648000
H	0.539651000	-3.662949000	2.445299000
O	1.108961000	-1.723022000	1.976931000
C	2.182550000	-1.830983000	2.912233000
H	2.487238000	-0.814071000	3.163345000
H	3.035887000	-2.368660000	2.485544000
H	1.829160000	-2.338796000	3.817704000
O	-0.833857000	-0.672939000	-0.251021000
C	-1.734340000	-1.604688000	-0.608591000
C	-1.214390000	-2.794533000	-1.175180000
C	0.202980000	-2.860960000	-1.677357000
H	0.348856000	-3.842433000	-2.157963000
H	0.348897000	-2.116294000	-2.472119000
C	-3.161714000	-1.484014000	-0.422978000
C	-3.907276000	-2.597206000	-0.811432000
H	-4.980248000	-2.508307000	-0.721476000
C	-3.412119000	-3.817851000	-1.286856000
C	-2.038042000	-3.878904000	-1.480749000
H	-1.575821000	-4.761159000	-1.912610000
C	-3.844996000	-0.156453000	0.084774000
C	-4.393200000	-4.996787000	-1.594816000
C	-5.402524000	-4.567261000	-2.696174000
H	-6.082483000	-5.383428000	-2.921724000
H	-4.878947000	-4.297592000	-3.608304000
H	-5.992044000	-3.714529000	-2.376977000
O	3.343201000	-0.651745000	0.062680000
C	4.208109000	-1.657653000	-0.018236000
C	3.875835000	-2.806922000	-0.765381000
C	2.585609000	-2.842862000	-1.532128000
H	2.578979000	-2.050391000	-2.295247000
H	2.519433000	-3.800737000	-2.074345000
C	5.464607000	-1.618105000	0.635453000
C	6.323128000	-2.711040000	0.513554000
H	7.283993000	-2.651764000	1.013702000
C	6.011185000	-3.866033000	-0.219473000
C	4.765130000	-3.882172000	-0.849168000
H	4.456107000	-4.739178000	-1.438666000
C	-5.171205000	-5.374926000	-0.303068000
H	-4.484448000	-5.679830000	0.480781000
H	-5.754850000	-4.536830000	0.062245000
H	-5.849996000	-6.199259000	-0.500557000

C	2. 018089000	5. 655478000	0. 179400000
H	1. 293444000	5. 996527000	0. 933766000
H	2. 919544000	5. 381630000	0. 742239000
Si	2. 406895000	7. 209577000	-0. 862614000
C	3. 799337000	6. 941467000	-2. 130387000
H	4. 709373000	6. 555115000	-1. 656163000
H	3. 499950000	6. 238347000	-2. 915498000
H	4. 055565000	7. 891100000	-2. 615724000
C	2. 952166000	8. 570260000	0. 349119000
H	3. 856871000	8. 275969000	0. 894548000
H	3. 171560000	9. 505649000	-0. 179098000
H	2. 169999000	8. 780246000	1. 088189000
C	0. 847588000	7. 780087000	-1. 784997000
H	0. 509271000	7. 028548000	-2. 507576000
H	0. 020988000	7. 974185000	-1. 091522000
H	1. 043141000	8. 706089000	-2. 338707000
N	1. 306904000	1. 525600000	-1. 783020000
C	2. 283477000	2. 475372000	-2. 061326000
C	0. 984193000	0. 653824000	-2. 772803000
C	3. 110864000	2. 275594000	-3. 217062000
C	2. 490625000	3. 623127000	-1. 271869000
C	1. 671619000	0. 505828000	-3. 960271000
H	0. 105392000	0. 042713000	-2. 566943000
C	2. 814493000	1. 315539000	-4. 149991000
H	3. 945758000	2. 953983000	-3. 371682000
C	1. 444170000	4. 416789000	-0. 536526000
H	1. 345428000	-0. 214478000	-4. 703133000
H	3. 428888000	1. 206222000	-5. 040223000
H	0. 910881000	3. 781776000	0. 179473000
H	0. 669478000	4. 779466000	-1. 243606000
C	-3. 148023000	1. 068174000	-0. 590783000
C	-2. 893102000	2. 255429000	0. 074546000
C	-2. 853206000	1. 009782000	-1. 960397000
C	-2. 388175000	3. 374920000	-0. 592324000
H	-3. 098674000	2. 345199000	1. 128727000
C	-2. 344581000	2. 100613000	-2. 641710000
H	-3. 049093000	0. 096011000	-2. 503668000
C	-2. 121237000	3. 290252000	-1. 945261000
H	-1. 738457000	4. 152692000	-2. 474595000
C	-3. 783784000	-0. 086161000	1. 647564000
C	-4. 555247000	0. 865475000	2. 331562000
C	-3. 056800000	-0. 987148000	2. 404770000
C	-4. 584855000	0. 924176000	3. 711396000
H	-5. 163601000	1. 557291000	1. 766611000

C	-3.070268000	-0.952634000	3.802911000
H	-2.484575000	-1.759200000	1.914878000
C	-3.830841000	0.004349000	4.444723000
H	-3.855626000	0.037192000	5.525876000
C	-5.372717000	-0.155170000	-0.289676000
C	-5.894240000	0.573887000	-1.343231000
C	-6.266863000	-0.919924000	0.475565000
C	-7.259939000	0.554395000	-1.645452000
H	-5.248610000	1.184992000	-1.953880000
C	-7.618987000	-0.958643000	0.197670000
H	-5.891193000	-1.495446000	1.309214000
C	-8.110955000	-0.211414000	-0.874854000
H	-9.169399000	-0.232952000	-1.098212000
C	-2.060314000	2.030629000	-4.140940000
H	-1.028559000	2.301581000	-4.349580000
H	-2.235551000	1.030013000	-4.522217000
H	-2.701554000	2.720348000	-4.685618000
C	-2.187457000	4.678884000	0.177933000
H	-1.553002000	4.522504000	1.046210000
H	-1.727321000	5.433709000	-0.450386000
H	-3.142160000	5.064172000	0.530423000
C	-5.430796000	1.968821000	4.436804000
H	-4.798966000	2.656631000	4.994758000
H	-6.021226000	2.545299000	3.732317000
H	-6.106705000	1.494121000	5.143836000
C	-2.246276000	-1.965967000	4.595093000
H	-1.182986000	-1.754106000	4.500716000
H	-2.503549000	-1.935741000	5.648888000
H	-2.417418000	-2.974786000	4.228453000
C	-7.783696000	1.380866000	-2.818549000
H	-8.859438000	1.277028000	-2.915430000
H	-7.552145000	2.434509000	-2.681228000
H	-7.323854000	1.060928000	-3.750788000
C	-8.572682000	-1.800666000	1.043010000
H	-9.061799000	-2.557678000	0.434079000
H	-8.040610000	-2.300331000	1.845870000
H	-9.349140000	-1.178901000	1.482513000
C	1.821669000	2.442095000	2.407761000
C	1.424948000	3.063973000	3.616333000
C	0.216395000	2.760747000	4.208691000
C	-0.629024000	1.837974000	3.584476000
C	-0.183609000	1.240739000	2.417392000
N	1.013667000	1.489440000	1.843896000
H	-0.078702000	3.248447000	5.134373000

H	2.087952000	3.801437000	4.059024000
H	-1.606940000	1.588460000	3.978874000
H	-0.825262000	0.534573000	1.892924000
C	3.046998000	2.891680000	1.797468000
H	3.514302000	3.716854000	2.331205000
C	3.600516000	2.517118000	0.606913000
H	4.554178000	2.945989000	0.314235000
H	3.359445000	1.589617000	0.107839000
H	3.345129000	4.213095000	-1.600133000
C	-3.639000000	-6.257419000	-2.091982000
H	-3.109577000	-6.059182000	-3.018075000
H	-2.925038000	-6.605075000	-1.352413000
H	-4.348671000	-7.057919000	-2.276345000
C	5.869408000	-0.358655000	1.436583000
C	7.040623000	-5.042560000	-0.300559000
C	6.979861000	0.435130000	0.705520000
H	6.655820000	0.707264000	-0.294565000
H	7.214597000	1.345958000	1.248941000
H	7.887584000	-0.154860000	0.621856000
C	6.298004000	-0.693450000	2.886199000
H	7.205739000	-1.288008000	2.902518000
H	6.485237000	0.221122000	3.441393000
H	5.519400000	-1.248985000	3.400258000
C	8.359819000	-4.534632000	-0.947134000
H	8.802832000	-3.737701000	-0.359680000
H	9.080378000	-5.344108000	-1.017295000
H	8.172561000	-4.156679000	-1.947591000
C	7.339715000	-5.573197000	1.129808000
H	8.049947000	-6.393537000	1.086066000
H	7.761289000	-4.794928000	1.756793000
H	6.430686000	-5.935124000	1.600666000
C	6.506840000	-6.223088000	-1.152937000
H	5.595046000	-6.632561000	-0.730551000
H	6.306787000	-5.911864000	-2.172933000
H	7.248173000	-7.015546000	-1.182886000
H	4.989246000	0.278515000	1.490469000

TS2^H_{syn}, $E_{(\text{SCF Done})} = -3320.173881 \text{ a.u.}$ IF = *i*186.79 cm⁻¹

Y	0.969298000	-0.039528000	0.355515000
N	0.884896000	2.528643000	0.126928000
C	0.967352000	2.920772000	-1.292938000
H	2.023705000	2.992341000	-1.563697000
H	0.521556000	3.915669000	-1.456803000
C	0.273027000	1.920541000	-2.207918000

H	-0.793268000	1.874672000	-1.998931000
H	0.408374000	2.217977000	-3.255697000
O	0.780214000	0.588323000	-2.028121000
C	1.817612000	0.235592000	-2.942363000
H	2.132061000	-0.778902000	-2.693458000
H	2.673467000	0.910999000	-2.851365000
H	1.423988000	0.255540000	-3.966069000
O	-1.162626000	0.393991000	0.241330000
C	-2.062346000	1.352331000	0.059938000
C	-1.676744000	2.706198000	0.223554000
C	-0.327479000	3.068245000	0.785363000
H	-0.250065000	4.168978000	0.802448000
H	-0.264338000	2.747599000	1.833794000
C	-3.425236000	1.089428000	-0.291682000
C	-4.285168000	2.175675000	-0.465446000
H	-5.321310000	1.963808000	-0.686342000
C	-3.900755000	3.519478000	-0.361729000
C	-2.574970000	3.750688000	-0.008266000
H	-2.206997000	4.763073000	0.123978000
C	-3.967145000	-0.394983000	-0.304786000
C	-4.949914000	4.653327000	-0.612261000
C	-6.108584000	4.529212000	0.416622000
H	-6.838708000	5.317247000	0.257681000
H	-5.729073000	4.615579000	1.430241000
H	-6.615813000	3.575002000	0.322754000
O	2.997563000	0.596522000	-0.102512000
C	3.790796000	1.654646000	-0.236611000
C	3.387121000	2.900976000	0.289039000
C	2.043064000	3.022699000	0.939454000
H	2.008588000	2.462448000	1.886493000
H	1.872802000	4.079876000	1.199371000
C	5.035018000	1.601751000	-0.918635000
C	5.841906000	2.740609000	-0.949238000
H	6.803185000	2.655241000	-1.445028000
C	5.478022000	3.970279000	-0.383266000
C	4.216658000	4.022100000	0.211292000
H	3.844495000	4.947944000	0.637589000
C	-5.523891000	4.523199000	-2.051130000
H	-4.730384000	4.607546000	-2.787478000
H	-6.018513000	3.568061000	-2.191113000
H	-6.248299000	5.309938000	-2.239706000
C	5.256718000	-3.635337000	-0.172035000
H	6.038244000	-3.203800000	-0.817011000
H	5.770957000	-3.903472000	0.763771000

Si	4.691492000	-5.244799000	-1.032687000
C	3.821488000	-6.447532000	0.150297000
H	4.457919000	-6.679234000	1.012792000
H	2.881044000	-6.029368000	0.523335000
H	3.594363000	-7.391779000	-0.359554000
C	6.251429000	-6.102354000	-1.708743000
H	6.952898000	-6.342447000	-0.900665000
H	5.997984000	-7.039660000	-2.218305000
H	6.777614000	-5.462794000	-2.427429000
C	3.538356000	-4.826039000	-2.483422000
H	2.626897000	-4.333460000	-2.126500000
H	4.031359000	-4.155066000	-3.197535000
H	3.243043000	-5.732431000	-3.024975000
N	1.175153000	-2.426539000	-0.073281000
C	1.852667000	-3.144704000	0.920814000
C	0.046750000	-2.984028000	-0.584495000
C	1.117811000	-4.150612000	1.635737000
C	3.213464000	-2.937978000	1.182981000
C	-0.557730000	-4.117817000	-0.090459000
H	-0.398960000	-2.445710000	-1.417523000
C	-0.043151000	-4.655419000	1.115442000
H	1.567541000	-4.578420000	2.527914000
C	4.198550000	-2.548596000	0.112354000
H	-1.437333000	-4.529391000	-0.570318000
H	-0.553035000	-5.478985000	1.610081000
H	4.728948000	-1.623307000	0.375299000
H	3.644676000	-2.315760000	-0.805109000
C	-3.727683000	-0.921550000	1.144304000
C	-2.943056000	-2.022642000	1.459236000
C	-4.310603000	-0.225186000	2.208916000
C	-2.771760000	-2.431425000	2.777052000
H	-2.451385000	-2.584376000	0.681132000
C	-4.150379000	-0.637167000	3.516181000
H	-4.909794000	0.651821000	2.003560000
C	-3.379244000	-1.756408000	3.824262000
C	-3.297763000	-1.259899000	-1.415737000
C	-3.625330000	-2.615667000	-1.532989000
C	-2.517480000	-0.705838000	-2.420952000
C	-3.156227000	-3.380520000	-2.580877000
H	-4.276437000	-3.071820000	-0.799492000
C	-2.041193000	-1.476419000	-3.476285000
H	-2.301773000	0.351191000	-2.408334000
C	-2.345813000	-2.824461000	-3.571186000
C	-5.487907000	-0.463508000	-0.680456000

C	-6.458677000	-1.025948000	0.132934000
C	-5.893889000	-0.025545000	-1.949074000
C	-7.783942000	-1.121404000	-0.281584000
H	-6.198454000	-1.409473000	1.107940000
C	-7.205456000	-0.116100000	-2.359295000
H	-5.159893000	0.392225000	-2.624840000
C	-8.181512000	-0.665998000	-1.525320000
C	1.577937000	-0.401482000	3.945765000
C	1.138622000	-0.239846000	5.287721000
C	-0.067687000	0.348531000	5.583758000
C	-0.888397000	0.756749000	4.522782000
C	-0.430363000	0.549220000	3.236097000
N	0.773751000	0.017628000	2.909336000
H	-0.379886000	0.480204000	6.616763000
H	1.796418000	-0.583036000	6.080886000
H	-1.866642000	1.196508000	4.683047000
H	-1.073593000	0.789680000	2.397788000
C	2.854697000	-1.011814000	3.747773000
H	3.272622000	-1.472603000	4.640927000
C	3.563991000	-1.112395000	2.580938000
H	3.606951000	-3.598294000	1.954702000
C	-4.321631000	6.063853000	-0.467583000
H	-3.936983000	6.222053000	0.534559000
H	-3.512200000	6.207662000	-1.175858000
H	-5.075538000	6.820664000	-0.660759000
C	5.492059000	0.305418000	-1.613105000
H	6.328797000	-0.132092000	-1.068840000
H	4.675988000	-0.407227000	-1.570752000
C	6.456653000	5.189209000	-0.458140000
H	4.579173000	-1.493717000	2.629834000
H	3.380866000	-0.468122000	1.726804000
H	-7.482221000	0.238032000	-3.344143000
H	-8.511622000	-1.565709000	0.385301000
H	-1.439992000	-1.006749000	-4.244032000
H	-3.431062000	-4.425847000	-2.642018000
H	-4.629193000	-0.081337000	4.312050000
H	-2.156694000	-3.298654000	2.980676000
C	-9.632609000	-0.763138000	-1.988115000
H	-10.247257000	-1.243507000	-1.233857000
H	-10.042505000	0.225291000	-2.183623000
H	-9.706874000	-1.338961000	-2.907698000
C	-1.818361000	-3.682252000	-4.717992000
H	-1.005353000	-4.320701000	-4.377115000
H	-2.600854000	-4.324911000	-5.112275000

H	-1.443280000	-3.061205000	-5.525165000
C	-3.226092000	-2.233035000	5.266262000
H	-2.279133000	-2.745539000	5.406173000
H	-3.273386000	-1.397992000	5.958797000
H	-4.023037000	-2.927157000	5.527719000
C	5.909685000	0.501656000	-3.087995000
H	6.780840000	1.143163000	-3.171570000
H	6.154831000	-0.457342000	-3.535546000
H	5.105649000	0.948956000	-3.664668000
C	7.790946000	4.826398000	0.252070000
H	8.269139000	3.976570000	-0.222911000
H	8.478216000	5.666406000	0.213991000
H	7.612614000	4.578406000	1.293964000
C	5.868321000	6.447958000	0.230724000
H	4.949085000	6.766074000	-0.250069000
H	5.663709000	6.261340000	1.279862000
H	6.580163000	7.265109000	0.167063000
C	6.744248000	5.538813000	-1.945391000
H	7.203433000	4.703308000	-2.462729000
H	5.824273000	5.795405000	-2.461917000
H	7.418562000	6.387697000	-2.009155000

TS2^H_{iso}, $E_{\text{(SCF Done)}} = -3320.178452$ a.u. IF = $i218.67$ cm⁻¹

Y	1.145314000	-0.229878000	0.030369000
N	1.144915000	-2.714642000	-0.675681000
C	1.067982000	-3.613293000	0.492890000
H	2.088508000	-3.895697000	0.769645000
H	0.523463000	-4.538277000	0.247343000
C	0.388846000	-2.934659000	1.671170000
H	-0.640510000	-2.669098000	1.432610000
H	0.390324000	-3.589749000	2.551848000
O	1.047263000	-1.699971000	2.001074000
C	2.143657000	-1.834454000	2.906048000
H	2.492481000	-0.825835000	3.131288000
H	2.962702000	-2.411454000	2.463421000
H	1.798542000	-2.313573000	3.830121000
O	-0.954919000	-0.651965000	-0.191425000
C	-1.886793000	-1.567095000	-0.511249000
C	-1.415871000	-2.785793000	-1.054810000
C	-0.016037000	-2.899475000	-1.592377000
H	0.088869000	-3.889345000	-2.066517000
H	0.130068000	-2.165568000	-2.397983000
C	-3.306146000	-1.389570000	-0.318905000
C	-4.095372000	-2.490526000	-0.648434000

H	-5.163916000	-2.359880000	-0.552264000
C	-3.646305000	-3.743753000	-1.085596000
C	-2.279290000	-3.853280000	-1.307841000
H	-1.854072000	-4.761761000	-1.723180000
C	-3.917912000	-0.000846000	0.104157000
C	-4.669015000	-4.900906000	-1.335598000
C	-5.676529000	-4.482383000	-2.442855000
H	-6.385172000	-5.284033000	-2.628682000
H	-5.155073000	-4.266282000	-3.370341000
H	-6.234363000	-3.598803000	-2.151810000
O	3.228721000	-0.717461000	-0.085592000
C	4.056402000	-1.755894000	-0.110252000
C	3.671953000	-2.945703000	-0.755167000
C	2.365842000	-2.989108000	-1.492024000
H	2.365004000	-2.239999000	-2.297467000
H	2.257694000	-3.973710000	-1.976694000
C	5.329891000	-1.698452000	0.513258000
C	6.143811000	-2.827782000	0.481663000
H	7.112394000	-2.770495000	0.962754000
C	5.775185000	-4.030577000	-0.146458000
C	4.523452000	-4.055960000	-0.760635000
H	4.177562000	-4.946935000	-1.274375000
C	-5.443860000	-5.201130000	-0.021690000
H	-4.758389000	-5.497207000	0.766656000
H	-5.995500000	-4.330280000	0.315667000
H	-6.151568000	-6.009655000	-0.178846000
C	2.013036000	5.611446000	0.286508000
H	1.327379000	5.948982000	1.078057000
H	2.920922000	5.281522000	0.806178000
Si	2.429548000	7.193110000	-0.703513000
C	3.854613000	6.958312000	-1.942473000
H	4.736703000	6.517015000	-1.463472000
H	3.563138000	6.312743000	-2.778359000
H	4.153964000	7.926639000	-2.361660000
C	2.953706000	8.511683000	0.563099000
H	3.839891000	8.191863000	1.124313000
H	3.196723000	9.460231000	0.069871000
H	2.152945000	8.706870000	1.286070000
C	0.895990000	7.800924000	-1.644687000
H	0.583832000	7.082432000	-2.411229000
H	0.047659000	7.958828000	-0.968517000
H	1.103540000	8.752589000	-2.148183000
N	1.123202000	1.546220000	-1.760260000
C	2.062228000	2.515204000	-2.096783000

C	0.742169000	0.680724000	-2.735424000
C	2.795655000	2.348821000	-3.320037000
C	2.331316000	3.648449000	-1.304296000
C	1.337578000	0.560587000	-3.974141000
H	-0.108298000	0.050886000	-2.473607000
C	2.444656000	1.396539000	-4.241629000
H	3.603635000	3.044803000	-3.529360000
C	1.363312000	4.425453000	-0.453095000
H	0.968428000	-0.157608000	-4.698587000
H	2.988950000	1.312398000	-5.179015000
H	0.857747000	3.765628000	0.260835000
H	0.557585000	4.850782000	-1.087118000
C	-3.208684000	1.100673000	-0.742041000
C	-2.738906000	2.301411000	-0.225383000
C	-3.084065000	0.903425000	-2.121704000
C	-2.197176000	3.276619000	-1.053912000
H	-2.797673000	2.502864000	0.833210000
C	-2.543985000	1.871390000	-2.944015000
H	-3.435291000	-0.021512000	-2.558869000
C	-2.096914000	3.084191000	-2.423885000
C	-3.773971000	0.212729000	1.644829000
C	-4.401550000	1.305062000	2.259131000
C	-3.155336000	-0.709804000	2.474790000
C	-4.393663000	1.464185000	3.628245000
H	-4.928717000	2.027200000	1.650280000
C	-3.151298000	-0.554039000	3.857578000
H	-2.693604000	-1.588858000	2.050497000
C	-3.768572000	0.530175000	4.456828000
C	-5.465185000	0.032497000	-0.166394000
C	-6.053107000	0.757874000	-1.191214000
C	-6.325319000	-0.679075000	0.682102000
C	-7.432340000	0.767396000	-1.374470000
H	-5.444990000	1.340301000	-1.866187000
C	-7.691068000	-0.673459000	0.500038000
H	-5.911192000	-1.246957000	1.503964000
C	-8.273111000	0.053904000	-0.539404000
C	1.997860000	2.367655000	2.377467000
C	1.729295000	2.972308000	3.629226000
C	0.563117000	2.700868000	4.313912000
C	-0.366418000	1.826358000	3.741912000
C	-0.042017000	1.239125000	2.531022000
N	1.111507000	1.456764000	1.864147000
H	0.364261000	3.176253000	5.271088000
H	2.455527000	3.673564000	4.029495000

H	-1.317935000	1.605929000	4.209407000
H	-0.750381000	0.564610000	2.052968000
C	3.179706000	2.796428000	1.673720000
H	3.722480000	3.586802000	2.188280000
C	3.604866000	2.448364000	0.425182000
H	4.536512000	2.863640000	0.052665000
H	3.285568000	1.546795000	-0.077017000
H	3.152902000	4.247967000	-1.693536000
C	-3.962274000	-6.204779000	-1.789064000
H	-3.441410000	-6.063008000	-2.730229000
H	-3.248063000	-6.543193000	-1.045435000
H	-4.699329000	-6.989379000	-1.928972000
C	5.731846000	-0.367634000	1.179572000
C	6.760519000	-5.247142000	-0.133969000
C	8.088786000	-4.847811000	-0.835860000
H	8.568815000	-4.020047000	-0.325151000
H	8.778007000	-5.687043000	-0.842052000
H	7.902166000	-4.551842000	-1.863671000
C	7.059021000	-5.661564000	1.334471000
H	7.737940000	-6.508852000	1.355794000
H	7.517390000	-4.848133000	1.886514000
H	6.143696000	-5.946438000	1.844448000
C	6.173195000	-6.477234000	-0.873620000
H	5.252345000	-6.813342000	-0.408312000
H	5.971964000	-6.249778000	-1.915262000
H	6.884552000	-7.296571000	-0.840181000
C	-9.787115000	0.058198000	-0.731899000
C	-3.797017000	0.696035000	5.974161000
C	-1.497939000	4.151019000	-3.335780000
H	-8.320932000	-1.238334000	1.175346000
H	-7.849250000	1.349221000	-2.186441000
H	-2.667626000	-1.303026000	4.471436000
H	-4.893103000	2.317905000	4.068468000
H	-1.858113000	4.206819000	-0.617438000
H	-2.476076000	1.688267000	-4.008746000
H	5.756159000	0.407172000	0.413995000
H	4.947180000	-0.076930000	1.878463000
H	-10.287475000	0.447622000	0.151807000
H	-10.066663000	0.673239000	-1.581016000
H	-3.127522000	-0.010746000	6.453785000
H	-3.499302000	1.701414000	6.260878000
H	-0.434260000	3.972956000	-3.482149000
H	-1.616517000	5.139968000	-2.904083000
C	7.081136000	-0.373524000	1.923897000

H	7.902965000	-0.584130000	1.246821000
H	7.255317000	0.600741000	2.371188000
H	7.090786000	-1.115440000	2.716549000
H	-10.157325000	-0.950011000	-0.903483000
H	-1.976899000	4.138861000	-4.310568000
H	-4.800256000	0.527003000	6.360116000

TS2^I_{syn}, $E_{(\text{SCF Done})} = -3713.091793$ a.u. **IF** = $i195.38$ cm⁻¹

Y	1.501991000	0.156458000	0.399106000
N	1.589661000	2.708076000	0.026548000
C	1.676506000	3.015791000	-1.413931000
H	2.731197000	3.002644000	-1.699466000
H	1.293166000	4.026821000	-1.627859000
C	0.905559000	2.014496000	-2.262418000
H	-0.158286000	2.053977000	-2.041414000
H	1.047040000	2.239252000	-3.327329000
O	1.324554000	0.664261000	-2.007164000
C	2.335138000	0.191825000	-2.898039000
H	2.580322000	-0.825803000	-2.590920000
H	3.234408000	0.811867000	-2.841132000
H	1.942694000	0.181793000	-3.922324000
O	-0.602505000	0.736241000	0.305040000
C	-1.435700000	1.746875000	0.086517000
C	-0.949509000	3.076125000	0.158497000
C	0.433818000	3.374081000	0.670004000
H	0.590020000	4.464959000	0.611900000
H	0.499067000	3.120162000	1.736319000
C	-2.823525000	1.567962000	-0.219491000
C	-3.602391000	2.703207000	-0.451360000
H	-4.654607000	2.556577000	-0.646193000
C	-3.118878000	4.018496000	-0.436722000
C	-1.773126000	4.169865000	-0.119929000
H	-1.327932000	5.157614000	-0.055904000
C	-3.472552000	0.128059000	-0.161825000
C	-4.086508000	5.210281000	-0.740152000
C	-5.230053000	5.235251000	0.312548000
H	-5.903953000	6.063947000	0.116361000
H	-4.824761000	5.355027000	1.312695000
H	-5.807024000	4.317074000	0.286438000
O	3.582927000	0.622973000	-0.081486000
C	4.439027000	1.617819000	-0.299969000
C	4.110440000	2.923294000	0.126810000
C	2.793195000	3.162921000	0.794941000
H	2.743435000	2.649791000	1.767293000

H	2.696229000	4.239776000	1.006635000
C	5.677211000	1.445195000	-0.974581000
C	6.523778000	2.543928000	-1.135630000
H	7.468843000	2.372554000	-1.639808000
C	6.223458000	3.837148000	-0.687883000
C	4.984610000	3.995241000	-0.066568000
H	4.664030000	4.969540000	0.287599000
C	-4.697569000	5.037022000	-2.159050000
H	-3.915096000	5.017289000	-2.911589000
H	-5.263842000	4.114787000	-2.232125000
H	-5.365767000	5.862902000	-2.384310000
C	5.342416000	-3.947498000	0.058361000
H	6.191796000	-3.649569000	-0.575916000
H	5.790417000	-4.224625000	1.024986000
Si	4.629060000	-5.525233000	-0.749330000
C	3.614184000	-6.583269000	0.456354000
H	4.200108000	-6.833760000	1.348880000
H	2.706587000	-6.062880000	0.779383000
H	3.312796000	-7.524858000	-0.018855000
C	6.109514000	-6.565788000	-1.341834000
H	6.766205000	-6.828398000	-0.503676000
H	5.774840000	-7.500663000	-1.807118000
H	6.712292000	-6.022514000	-2.079301000
C	3.558008000	-5.058439000	-2.247276000
H	2.681170000	-4.480213000	-1.934819000
H	4.124968000	-4.454898000	-2.966570000
H	3.202716000	-5.954930000	-2.768891000
N	1.454784000	-2.239847000	-0.021743000
C	2.014319000	-3.002500000	1.009886000
C	0.313386000	-2.703121000	-0.592961000
C	1.163811000	-3.938872000	1.687007000
C	3.381011000	-2.917768000	1.321434000
C	-0.401860000	-3.786602000	-0.134969000
H	-0.044056000	-2.131528000	-1.445993000
C	0.000666000	-4.357416000	1.097646000
H	1.528440000	-4.399070000	2.601635000
C	4.421997000	-2.723150000	0.248062000
H	-1.282762000	-4.130230000	-0.663368000
H	-0.595414000	-5.141619000	1.558701000
H	5.059847000	-1.856898000	0.464158000
H	3.914616000	-2.484860000	-0.694827000
C	-3.175294000	-0.419693000	1.269103000
C	-2.602362000	-1.657823000	1.534540000
C	-3.523201000	0.360524000	2.372563000

C	-2.430746000	-2.108135000	2.834696000
H	-2.286927000	-2.297878000	0.726799000
C	-3.358862000	-0.093117000	3.669653000
H	-3.955725000	1.339518000	2.214835000
C	-2.819791000	-1.349215000	3.934265000
C	-2.952921000	-0.789854000	-1.310850000
C	-3.450712000	-2.092441000	-1.444408000
C	-2.134077000	-0.329028000	-2.327669000
C	-3.107524000	-2.888360000	-2.514961000
H	-4.138905000	-2.479012000	-0.704922000
C	-1.784703000	-1.134376000	-3.409246000
H	-1.781873000	0.690014000	-2.309782000
C	-2.255317000	-2.431492000	-3.526965000
C	-5.021479000	0.182679000	-0.409641000
C	-5.975563000	-0.169672000	0.536555000
C	-5.496329000	0.538397000	-1.673762000
C	-7.330006000	-0.145264000	0.240313000
H	-5.674813000	-0.478770000	1.525934000
C	-6.846583000	0.566809000	-1.967959000
H	-4.791182000	0.800209000	-2.451030000
C	-7.802306000	0.226684000	-1.013256000
C	2.172495000	-0.013778000	3.979421000
C	1.833706000	0.349971000	5.311073000
C	0.713419000	1.096864000	5.588620000
C	-0.130141000	1.454072000	4.526481000
C	0.230917000	1.056491000	3.253751000
N	1.362545000	0.378955000	2.937974000
H	0.480627000	1.385126000	6.610703000
H	2.499126000	0.032113000	6.108437000
H	-1.052737000	2.003291000	4.679315000
H	-0.432923000	1.258559000	2.421335000
C	3.350206000	-0.800549000	3.793555000
H	3.741366000	-1.243438000	4.707748000
C	3.994098000	-1.077129000	2.616619000
H	3.677874000	-3.581204000	2.132683000
C	-3.353164000	6.576015000	-0.692506000
H	-2.937394000	6.764897000	0.291736000
H	-2.549999000	6.616003000	-1.421095000
H	-4.052973000	7.374202000	-0.919738000
C	6.100206000	0.059156000	-1.513064000
C	7.245027000	5.002208000	-0.906381000
H	4.947648000	-1.593077000	2.668032000
H	3.878941000	-0.461435000	1.730001000
C	7.329612000	-0.488772000	-0.747197000

H	7.129587000	-0.531878000	0.318886000
H	7.575272000	-1.489523000	-1.089835000
H	8.196798000	0.145244000	-0.904387000
C	6.385352000	0.084567000	-3.035617000
H	7.246109000	0.704608000	-3.264579000
H	6.589739000	-0.920129000	-3.394248000
H	5.533820000	0.473472000	-3.585066000
C	7.506538000	5.189638000	-2.427329000
H	8.210851000	5.999818000	-2.591391000
H	7.919736000	4.288711000	-2.867962000
H	6.583772000	5.430524000	-2.946428000
C	8.582976000	4.659455000	-0.193075000
H	9.299658000	5.463783000	-0.330315000
H	8.422713000	4.523298000	0.872111000
H	9.016924000	3.748508000	-0.591003000
C	6.722102000	6.345847000	-0.335187000
H	5.801313000	6.648667000	-0.822863000
H	6.541198000	6.274335000	0.732297000
H	7.460531000	7.124429000	-0.499632000
H	-7.145171000	0.856447000	-2.964181000
H	-8.026750000	-0.429953000	1.016479000
H	-1.146547000	-0.710212000	-4.169631000
H	-3.522600000	-3.885080000	-2.571287000
H	-3.671704000	0.550759000	4.477797000
H	-1.998029000	-3.087818000	2.979891000
C	-9.328360000	0.240139000	-1.295931000
C	-9.654257000	0.685311000	-2.745387000
H	-9.291840000	1.689471000	-2.939312000
H	-9.213710000	0.011073000	-3.472384000
H	-10.729701000	0.681879000	-2.892492000
C	-10.027509000	1.226673000	-0.318395000
H	-11.095886000	1.250804000	-0.510795000
H	-9.876403000	0.929807000	0.713829000
H	-9.635450000	2.231247000	-0.445424000
C	-9.906702000	-1.187873000	-1.086701000
H	-9.427964000	-1.894818000	-1.757529000
H	-9.754277000	-1.527746000	-0.068018000
H	-10.973403000	-1.193602000	-1.289621000
C	-1.905897000	-3.360504000	-4.719976000
C	-0.927800000	-2.689979000	-5.719456000
H	-1.360357000	-1.795016000	-6.154392000
H	0.006541000	-2.424764000	-5.235561000
H	-0.704087000	-3.380590000	-6.526415000
C	-1.237838000	-4.660749000	-4.190547000

H	-1.904388000	-5.204271000	-3.529946000
H	-0.978876000	-5.311980000	-5.019850000
H	-0.329744000	-4.428055000	-3.642646000
C	-3.207959000	-3.726471000	-5.487170000
H	-3.908726000	-4.247304000	-4.843567000
H	-3.692500000	-2.831284000	-5.865202000
H	-2.977822000	-4.371661000	-6.329683000
C	-2.679757000	-1.932035000	5.366243000
C	-3.058316000	-0.900540000	6.460995000
H	-2.923621000	-1.345797000	7.441749000
H	-2.430071000	-0.017905000	6.402478000
H	-4.095135000	-0.593840000	6.372583000
C	-1.216170000	-2.389800000	5.619632000
H	-0.917939000	-3.164466000	4.922208000
H	-0.530852000	-1.555189000	5.515084000
H	-1.119332000	-2.786640000	6.625631000
C	-3.627460000	-3.157587000	5.504868000
H	-4.659140000	-2.863320000	5.337252000
H	-3.372158000	-3.929541000	4.786524000
H	-3.551061000	-3.581813000	6.501575000
H	5.266017000	-0.615861000	-1.342825000

TS2^I_{iso}, $E_{\text{(SCF Done)}} = -3713.098254$ a.u. IF = $i274.80$ cm⁻¹

Y	1.659036000	-0.385302000	-0.087180000
N	1.702092000	-2.785850000	-0.988300000
C	1.608528000	-3.769996000	0.107786000
H	2.626690000	-4.045858000	0.398904000
H	1.098646000	-4.687798000	-0.224313000
C	0.868518000	-3.203267000	1.310569000
H	-0.161735000	-2.958369000	1.057420000
H	0.866475000	-3.924728000	2.137527000
O	1.467873000	-1.975200000	1.759788000
C	2.511898000	-2.139321000	2.719906000
H	2.838220000	-1.138891000	3.007392000
H	3.360330000	-2.690078000	2.300104000
H	2.118794000	-2.660189000	3.601059000
O	-0.426747000	-0.776095000	-0.441554000
C	-1.342175000	-1.689402000	-0.812537000
C	-0.841661000	-2.858633000	-1.432052000
C	0.568013000	-2.901904000	-1.949165000
H	0.700660000	-3.842138000	-2.509381000
H	0.720816000	-2.092268000	-2.678314000
C	-2.763981000	-1.566021000	-0.593706000
C	-3.522587000	-2.660539000	-1.009229000

H	-4.593645000	-2.567512000	-0.900373000
C	-3.044372000	-3.867084000	-1.537352000
C	-1.675624000	-3.927410000	-1.763917000
H	-1.226555000	-4.793186000	-2.240843000
C	-3.426987000	-0.244120000	-0.048986000
C	-4.039018000	-5.027947000	-1.869340000
C	-5.062418000	-4.554198000	-2.939126000
H	-5.751863000	-5.357539000	-3.181297000
H	-4.551404000	-4.257188000	-3.849894000
H	-5.640457000	-3.708817000	-2.581643000
O	3.746713000	-0.893069000	-0.087164000
C	4.585082000	-1.917878000	-0.205398000
C	4.231446000	-3.015968000	-1.016167000
C	2.948037000	-2.971437000	-1.791458000
H	2.970226000	-2.138500000	-2.510533000
H	2.856691000	-3.895524000	-2.386027000
C	5.831726000	-1.951709000	0.467463000
C	6.658679000	-3.062815000	0.298675000
H	7.612526000	-3.059888000	0.815420000
C	6.324633000	-4.167398000	-0.499250000
C	5.088402000	-4.112411000	-1.145770000
H	4.761865000	-4.927753000	-1.783030000
C	-4.799112000	-5.444483000	-0.578771000
H	-4.102248000	-5.780562000	0.183097000
H	-5.370778000	-4.615417000	-0.175839000
H	-5.486904000	-6.257010000	-0.793255000
C	2.731388000	5.386810000	0.786194000
H	2.025593000	5.687571000	1.574920000
H	3.587548000	4.948374000	1.312835000
Si	3.300640000	7.030085000	-0.006232000
C	4.598369000	6.808181000	-1.379653000
H	5.465454000	6.235731000	-1.029451000
H	4.179472000	6.293316000	-2.251442000
H	4.960969000	7.787284000	-1.715841000
C	4.073232000	8.071399000	1.385110000
H	4.949586000	7.570583000	1.813681000
H	4.398339000	9.049792000	1.012097000
H	3.357526000	8.245384000	2.197314000
C	1.810739000	7.959248000	-0.729943000
H	1.367711000	7.414764000	-1.571288000
H	1.027991000	8.107198000	0.023112000
H	2.112533000	8.947151000	-1.097725000
N	1.752346000	1.574936000	-1.692868000
C	2.750086000	2.522924000	-1.876041000

C	1. 384304000	0. 833920000	-2. 769686000
C	3. 531565000	2. 459012000	-3. 075090000
C	3. 042954000	3. 542776000	-0. 937557000
C	2. 039273000	0. 816733000	-3. 985241000
H	0. 497591000	0. 218076000	-2. 613604000
C	3. 188640000	1. 625790000	-4. 110710000
H	4. 375000000	3. 137256000	-3. 172795000
C	2. 058883000	4. 317995000	-0. 098556000
H	1. 680912000	0. 193963000	-4. 798189000
H	3. 774079000	1. 618933000	-5. 026757000
H	1. 455612000	3. 642772000	0. 516867000
H	1. 331303000	4. 846839000	-0. 748529000
C	-2. 785862000	0. 970396000	-0. 790313000
C	-2. 503844000	2. 188502000	-0. 192431000
C	-2. 577526000	0. 883611000	-2. 172819000
C	-2. 088284000	3. 287039000	-0. 940362000
H	-2. 624473000	2. 317035000	0. 872054000
C	-2. 165306000	1. 971356000	-2. 911502000
H	-2. 777260000	-0. 049023000	-2. 682607000
C	-1. 936536000	3. 215963000	-2. 316452000
C	-3. 296436000	-0. 171923000	1. 506640000
C	-4. 014176000	0. 789307000	2. 231256000
C	-2. 600907000	-1. 113657000	2. 245977000
C	-4. 025080000	0. 795573000	3. 608877000
H	-4. 606125000	1. 524208000	1. 702913000
C	-2. 610862000	-1. 107806000	3. 638633000
H	-2. 062767000	-1. 901150000	1. 740873000
C	-3. 325850000	-0. 161655000	4. 353625000
C	-4. 973253000	-0. 255505000	-0. 335835000
C	-5. 575189000	0. 482543000	-1. 348639000
C	-5. 820658000	-1. 031316000	0. 456953000
C	-6. 944705000	0. 443000000	-1. 556669000
H	-4. 980076000	1. 111371000	-1. 992746000
C	-7. 187274000	-1. 073454000	0. 247385000
H	-5. 405628000	-1. 621497000	1. 262301000
C	-7. 786860000	-0. 334357000	-0. 768400000
C	2. 301302000	2. 053801000	2. 455315000
C	1. 874468000	2. 616499000	3. 681437000
C	0. 563797000	2. 488388000	4. 095519000
C	-0. 340862000	1. 799803000	3. 281486000
C	0. 145712000	1. 208200000	2. 126650000
N	1. 433867000	1. 279646000	1. 730213000
H	0. 237152000	2. 943891000	5. 027099000
H	2. 587990000	3. 191601000	4. 264445000

H	-1.391769000	1.715761000	3.527470000
H	-0.529944000	0.663490000	1.463722000
C	3.603593000	2.412705000	1.958202000
H	4.144357000	3.096644000	2.609328000
C	4.116523000	2.178638000	0.710144000
H	5.111489000	2.547986000	0.477818000
H	3.803018000	1.349280000	0.094585000
H	3.917709000	4.125733000	-1.222669000
C	-3.301789000	-6.275895000	-2.420975000
H	-2.787663000	-6.050502000	-3.349465000
H	-2.577023000	-6.651664000	-1.706062000
H	-4.019695000	-7.065788000	-2.618674000
C	6.263678000	-0.752904000	1.343666000
C	7.319623000	-5.369045000	-0.627395000
C	7.413406000	0.040854000	0.676088000
H	7.117327000	0.378606000	-0.312581000
H	7.668402000	0.911804000	1.273079000
H	8.302317000	-0.574496000	0.574867000
C	6.655086000	-1.181700000	2.778985000
H	7.542574000	-1.806312000	2.776993000
H	6.861724000	-0.305791000	3.387077000
H	5.849705000	-1.738211000	3.248769000
C	8.664622000	-4.868283000	-1.224481000
H	9.120972000	-4.117991000	-0.587881000
H	9.361654000	-5.694767000	-1.326653000
H	8.506487000	-4.431818000	-2.205968000
C	7.577432000	-5.984220000	0.776917000
H	8.263446000	-6.822568000	0.700403000
H	8.010992000	-5.253846000	1.451547000
H	6.649815000	-6.342530000	1.213005000
C	6.765609000	-6.485189000	-1.550628000
H	5.835148000	-6.888885000	-1.164997000
H	6.592012000	-6.113538000	-2.555131000
H	7.483588000	-7.297076000	-1.612281000
H	5.404934000	-0.089683000	1.419434000
H	-7.782480000	-1.696946000	0.897344000
H	-7.355950000	1.041288000	-2.357812000
H	-2.057944000	-1.880792000	4.150773000
H	-4.608287000	1.551307000	4.116454000
H	-2.041721000	1.853239000	-3.978992000
H	-1.906786000	4.213268000	-0.415891000
C	-9.314828000	-0.345153000	-1.040284000
C	-10.080085000	-1.271488000	-0.059693000
H	-9.742430000	-2.299120000	-0.144800000

H	-9.951778000	-0.948144000	0.968037000
H	-11.140514000	-1.246076000	-0.290043000
C	-9.579670000	-0.848103000	-2.487500000
H	-10.646654000	-0.867340000	-2.687965000
H	-9.109444000	-0.201190000	-3.220188000
H	-9.189769000	-1.852904000	-2.619260000
C	-9.878564000	1.095510000	-0.884911000
H	-9.413827000	1.776969000	-1.589248000
H	-10.949301000	1.100233000	-1.065268000
H	-9.700094000	1.468344000	0.119145000
C	-3.408275000	-0.146385000	5.903698000
C	-2.545971000	-1.262516000	6.548673000
H	-2.881730000	-2.247096000	6.240531000
H	-1.499582000	-1.153476000	6.282829000
H	-2.626420000	-1.203759000	7.629538000
C	-4.885812000	-0.362629000	6.337928000
H	-5.525336000	0.426549000	5.957327000
H	-5.257387000	-1.312436000	5.965443000
H	-4.961279000	-0.367590000	7.421116000
C	-2.910059000	1.221830000	6.448069000
H	-1.872866000	1.386970000	6.173954000
H	-3.502299000	2.041766000	6.056652000
H	-2.981929000	1.240418000	7.531254000
C	-1.560018000	4.435027000	-3.200045000
C	-1.465944000	5.746276000	-2.378189000
H	-1.218625000	6.571261000	-3.038747000
H	-2.410456000	5.973526000	-1.894555000
H	-0.694896000	5.680910000	-1.618994000
C	-2.650622000	4.636625000	-4.291085000
H	-2.413006000	5.504225000	-4.899075000
H	-2.718940000	3.775489000	-4.946580000
H	-3.623022000	4.796732000	-3.835099000
C	-0.189342000	4.181202000	-3.886081000
H	0.588883000	4.042274000	-3.142434000
H	-0.224780000	3.295666000	-4.511553000
H	0.079302000	5.027923000	-4.510576000

TS2^J_{syn}, $E_{\text{(SCF Done)}} = -3438.060269$ a.u. **IF** = *i*158.93 cm⁻¹

Y	1.194507000	-0.072269000	0.375058000
N	1.208502000	2.489377000	0.151027000
C	1.309948000	2.881081000	-1.268255000
H	2.369598000	2.928059000	-1.531390000
H	0.889747000	3.886584000	-1.433276000
C	0.596980000	1.901430000	-2.193844000

H	-0.472594000	1.876120000	-1.996146000
H	0.748612000	2.203244000	-3.238343000
O	1.069723000	0.554835000	-2.022825000
C	2.147034000	0.215597000	-2.897148000
H	2.427196000	-0.815482000	-2.678024000
H	3.010506000	0.866208000	-2.733410000
H	1.808361000	0.287586000	-3.937388000
O	-0.935029000	0.435833000	0.267555000
C	-1.780924000	1.432649000	0.024321000
C	-1.331245000	2.768715000	0.178444000
C	0.006386000	3.062114000	0.798506000
H	0.127550000	4.157785000	0.847349000
H	0.025654000	2.710442000	1.838468000
C	-3.140683000	1.242051000	-0.383609000
C	-3.915239000	2.375737000	-0.648945000
H	-4.949744000	2.219463000	-0.917909000
C	-3.455306000	3.696020000	-0.574695000
C	-2.144243000	3.858542000	-0.138531000
H	-1.722623000	4.850039000	-0.008868000
C	-3.829594000	-0.177328000	-0.287558000
C	-4.412083000	4.880516000	-0.935281000
C	-5.636849000	4.874060000	0.021962000
H	-6.302237000	5.699500000	-0.213109000
H	-5.314824000	4.978932000	1.053575000
H	-6.199473000	3.950991000	-0.067530000
O	3.244379000	0.489085000	-0.081201000
C	4.080771000	1.517561000	-0.197115000
C	3.719347000	2.773043000	0.337602000
C	2.374016000	2.942242000	0.974492000
H	2.310141000	2.384362000	1.921318000
H	2.239146000	4.004980000	1.232705000
C	5.329237000	1.425863000	-0.867391000
C	6.179600000	2.533414000	-0.874351000
H	7.142539000	2.416404000	-1.360193000
C	5.857597000	3.768987000	-0.297151000
C	4.591889000	3.862234000	0.282750000
H	4.250183000	4.796634000	0.715742000
C	-4.904590000	4.723185000	-2.401321000
H	-4.064062000	4.727668000	-3.088687000
H	-5.448646000	3.794302000	-2.534453000
H	-5.565335000	5.543232000	-2.666320000
C	5.213876000	-3.845216000	-0.510671000
H	5.936234000	-3.415250000	-1.222725000
H	5.824513000	-4.249956000	0.310810000

Si	4.377587000	-5.305763000	-1.413283000
C	3.571024000	-6.542539000	-0.221159000
H	4.301761000	-6.916917000	0.505894000
H	2.746432000	-6.083527000	0.333740000
H	3.173935000	-7.405582000	-0.769507000
C	5.731617000	-6.222668000	-2.389395000
H	6.512674000	-6.601641000	-1.719319000
H	5.314975000	-7.079872000	-2.931786000
H	6.212956000	-5.565176000	-3.123201000
C	3.076542000	-4.646286000	-2.631846000
H	2.283048000	-4.111118000	-2.098051000
H	3.528733000	-3.956618000	-3.355414000
H	2.613922000	-5.465634000	-3.194605000
N	1.265496000	-2.507378000	0.285550000
C	2.074367000	-3.252624000	1.153978000
C	-0.001569000	-2.954368000	0.076821000
C	1.429769000	-4.193053000	2.030313000
C	3.462365000	-3.119951000	1.190813000
C	-0.591741000	-4.000488000	0.746703000
H	-0.572468000	-2.396671000	-0.660355000
C	0.139941000	-4.587380000	1.808464000
H	2.030684000	-4.654918000	2.809014000
C	4.314857000	-2.710437000	0.027325000
H	-1.599488000	-4.314187000	0.505057000
H	-0.313448000	-5.355837000	2.430387000
H	4.966057000	-1.867971000	0.300225000
H	3.669618000	-2.335160000	-0.775635000
C	-3.839936000	-0.477705000	1.245282000
C	-3.135261000	-1.504140000	1.846000000
C	-4.568302000	0.391852000	2.072730000
C	-3.175747000	-1.699083000	3.233240000
H	-2.541317000	-2.179643000	1.251083000
C	-4.623969000	0.220817000	3.440069000
H	-5.105732000	1.215450000	1.624912000
C	-3.923808000	-0.843092000	4.015002000
H	-3.964929000	-0.989910000	5.086066000
C	-3.144367000	-1.264012000	-1.170196000
C	-3.548232000	-2.596264000	-1.058211000
C	-2.300499000	-0.922890000	-2.221306000
C	-3.101168000	-3.568076000	-1.940079000
H	-4.247365000	-2.875004000	-0.282921000
C	-1.841711000	-1.880740000	-3.124234000
H	-2.025936000	0.110464000	-2.370149000
C	-2.241000000	-3.199450000	-2.970122000

H	-1.894358000	-3.948500000	-3.669824000
C	-5.286300000	-0.173799000	-0.871307000
C	-6.377984000	-0.662386000	-0.176633000
C	-5.483213000	0.225042000	-2.201623000
C	-7.647953000	-0.725855000	-0.759854000
H	-6.264126000	-1.012403000	0.837904000
C	-6.726255000	0.174912000	-2.799965000
H	-4.638813000	0.579383000	-2.775388000
C	-7.813594000	-0.300885000	-2.062364000
H	-8.791196000	-0.344849000	-2.523773000
C	-5.438970000	1.165805000	4.320902000
H	-6.258978000	0.634953000	4.799700000
H	-4.820803000	1.593216000	5.106743000
H	-5.856495000	1.977958000	3.734824000
C	-2.402925000	-2.857564000	3.860232000
H	-1.347576000	-2.801583000	3.605665000
H	-2.497671000	-2.844092000	4.941097000
H	-2.778185000	-3.811330000	3.496703000
C	-3.561254000	-5.019004000	-1.810486000
H	-4.125511000	-5.322565000	-2.689460000
H	-2.708130000	-5.686816000	-1.718032000
H	-4.193855000	-5.148428000	-0.938522000
C	-0.934132000	-1.489623000	-4.288876000
H	0.049820000	-1.939804000	-4.179377000
H	-1.350416000	-1.833101000	-5.232784000
H	-0.814164000	-0.412700000	-4.340605000
C	-8.824471000	-1.265680000	0.051308000
H	-9.731864000	-1.277215000	-0.543564000
H	-8.625090000	-2.279165000	0.391410000
H	-9.000497000	-0.651099000	0.931260000
C	-6.923630000	0.624492000	-4.246336000
H	-7.615358000	1.462337000	-4.298751000
H	-5.981649000	0.932062000	-4.688343000
H	-7.336468000	-0.182166000	-4.847485000
C	1.875803000	-0.458619000	3.949354000
C	1.449077000	-0.305829000	5.295925000
C	0.242030000	0.274038000	5.609348000
C	-0.590291000	0.691342000	4.562117000
C	-0.138695000	0.504827000	3.269351000
N	1.062192000	-0.022526000	2.928228000
H	-0.061277000	0.390845000	6.646787000
H	2.112811000	-0.656259000	6.080831000
H	-1.570427000	1.121893000	4.735615000
H	-0.786544000	0.758434000	2.437343000

C	3.150805000	-1.079187000	3.742327000
H	3.573577000	-1.520323000	4.643194000
C	3.853404000	-1.216322000	2.578307000
H	3.948556000	-3.782107000	1.906530000
C	-3.703272000	6.254017000	-0.807316000
H	-3.373474000	6.432961000	0.210755000
H	-2.842762000	6.314453000	-1.465659000
H	-4.392100000	7.047185000	-1.080917000
C	5.750222000	0.124694000	-1.575690000
C	6.883756000	4.949534000	-0.344776000
H	4.862146000	-1.614454000	2.625926000
H	3.649435000	-0.625984000	1.691573000
C	6.187626000	0.327197000	-3.044094000
H	7.079665000	0.941287000	-3.111208000
H	6.406129000	-0.633292000	-3.502099000
H	5.403934000	0.807634000	-3.622098000
C	7.203419000	5.305590000	-1.823904000
H	7.910927000	6.128254000	-1.868675000
H	7.636385000	4.459172000	-2.346087000
H	6.300713000	5.604106000	-2.348313000
C	8.193718000	4.525890000	0.376932000
H	8.913705000	5.338685000	0.357823000
H	7.992695000	4.272414000	1.413362000
H	8.644251000	3.663805000	-0.102987000
C	6.336126000	6.221717000	0.352866000
H	5.436136000	6.581368000	-0.135017000
H	6.111166000	6.030373000	1.396976000
H	7.079994000	7.011123000	0.308281000
H	4.912538000	-0.562693000	-1.550696000
H	6.567873000	-0.346136000	-1.030324000

TS2^J_{iso}, $E_{(\text{SCF Done})} = -3438.066214$ a.u. IF = $i226.87$ cm⁻¹

Y	1.331808000	-0.203703000	0.049185000
N	1.422702000	-2.657418000	-0.727330000
C	1.348728000	-3.591486000	0.412889000
H	2.371813000	-3.840296000	0.711144000
H	0.850049000	-4.530317000	0.125577000
C	0.609416000	-2.976905000	1.589790000
H	-0.421392000	-2.743989000	1.326950000
H	0.609726000	-3.660516000	2.448487000
O	1.206675000	-1.728900000	1.980273000
C	2.279271000	-1.849788000	2.915169000
H	2.577968000	-0.836118000	3.185833000
H	3.135638000	-2.376641000	2.480703000

H	1. 926628000	-2. 374589000	3. 811125000
O	-0. 745937000	-0. 672182000	-0. 246046000
C	-1. 647159000	-1. 599834000	-0. 613229000
C	-1. 126505000	-2. 787157000	-1. 184424000
C	0. 292747000	-2. 851782000	-1. 680555000
H	0. 437910000	-3. 828230000	-2. 171478000
H	0. 444604000	-2. 098351000	-2. 466017000
C	-3. 075451000	-1. 478635000	-0. 433589000
C	-3. 820329000	-2. 588950000	-0. 831660000
H	-4. 893551000	-2. 499380000	-0. 745834000
C	-3. 324658000	-3. 807429000	-1. 311865000
C	-1. 949864000	-3. 868827000	-1. 500110000
H	-1. 486595000	-4. 748908000	-1. 935254000
C	-3. 760965000	-0. 154307000	0. 079771000
C	-4. 305743000	-4. 983407000	-1. 630834000
C	-5. 309658000	-4. 546469000	-2. 734212000
H	-5. 989587000	-5. 360524000	-2. 967360000
H	-4. 781717000	-4. 272314000	-3. 642480000
H	-5. 899559000	-3. 694821000	-2. 412829000
O	3. 433208000	-0. 634440000	0. 018689000
C	4. 290160000	-1. 647704000	-0. 031579000
C	3. 957844000	-2. 816017000	-0. 742457000
C	2. 674002000	-2. 864517000	-1. 518058000
H	2. 673883000	-2. 084391000	-2. 293371000
H	2. 608192000	-3. 831659000	-2. 043837000
C	5. 544275000	-1. 584812000	0. 629609000
C	6. 392945000	-2. 686889000	0. 565867000
H	7. 346485000	-2. 625093000	1. 075602000
C	6. 077149000	-3. 867577000	-0. 129201000
C	4. 842651000	-3. 899372000	-0. 777058000
H	4. 536961000	-4. 774342000	-1. 341263000
C	-5. 089921000	-5. 367903000	-0. 344706000
H	-4. 407011000	-5. 678017000	0. 440459000
H	-5. 674231000	-4. 531200000	0. 022727000
H	-5. 768767000	-6. 190319000	-0. 549849000
C	2. 108954000	5. 660951000	0. 228246000
H	1. 381954000	6. 003488000	0. 979638000
H	3. 009140000	5. 389539000	0. 794422000
Si	2. 499519000	7. 211797000	-0. 817939000
C	3. 892180000	6. 938454000	-2. 084304000
H	4. 802996000	6. 556611000	-1. 607908000
H	3. 593848000	6. 229961000	-2. 864976000
H	4. 146704000	7. 885565000	-2. 575431000
C	3. 045169000	8. 576142000	0. 389485000

H	3.949687000	8.283265000	0.935985000
H	3.265005000	9.509712000	-0.141758000
H	2.263017000	8.788884000	1.127785000
C	0.941041000	7.780304000	-1.742940000
H	0.602463000	7.026487000	-2.463013000
H	0.114286000	7.977509000	-1.050526000
H	1.137546000	8.704187000	-2.299843000
N	1.396976000	1.541275000	-1.755667000
C	2.386262000	2.483380000	-2.012325000
C	1.081768000	0.677903000	-2.755148000
C	3.227974000	2.285276000	-3.157839000
C	2.590954000	3.623853000	-1.211253000
C	1.784938000	0.532535000	-3.933721000
H	0.196359000	0.071334000	-2.564894000
C	2.936730000	1.334308000	-4.101601000
H	4.070886000	2.957322000	-3.295679000
C	1.538756000	4.419785000	-0.486390000
H	1.464125000	-0.180486000	-4.685890000
H	3.562747000	1.225976000	-4.983824000
H	1.001720000	3.787536000	0.229470000
H	0.767807000	4.779193000	-1.198907000
C	-3.057478000	1.075083000	-0.580010000
C	-2.803792000	2.255472000	0.097861000
C	-2.755169000	1.028883000	-1.948470000
C	-2.293370000	3.380264000	-0.555795000
H	-3.014527000	2.335597000	1.151802000
C	-2.241483000	2.125291000	-2.616913000
H	-2.949382000	0.120435000	-2.501202000
C	-2.019976000	3.307986000	-1.908166000
H	-1.633270000	4.174778000	-2.427428000
C	-3.712300000	-0.097864000	1.643583000
C	-4.486414000	0.850043000	2.329667000
C	-2.995309000	-1.008652000	2.398646000
C	-4.528345000	0.895601000	3.709718000
H	-5.087313000	1.549327000	1.765923000
C	-3.021440000	-0.987636000	3.796820000
H	-2.421565000	-1.778107000	1.906421000
C	-3.784470000	-0.034070000	4.440927000
H	-3.819082000	-0.011637000	5.522076000
C	-5.285962000	-0.147701000	-0.306371000
C	-5.798332000	0.589722000	-1.358625000
C	-6.187376000	-0.916138000	0.446609000
C	-7.161705000	0.574782000	-1.671388000
H	-5.147191000	1.204139000	-1.959979000

C	-7.537414000	-0.950500000	0.158165000
H	-5.819263000	-1.498115000	1.279123000
C	-8.019930000	-0.194932000	-0.912780000
H	-9.076673000	-0.213006000	-1.144342000
C	-1.950524000	2.069234000	-4.115448000
H	-0.920484000	2.351041000	-4.317889000
H	-2.115394000	1.070074000	-4.505081000
H	-2.595841000	2.757305000	-4.657469000
C	-2.093966000	4.676471000	0.227777000
H	-1.465903000	4.510114000	1.098838000
H	-1.627281000	5.435601000	-0.390443000
H	-3.049869000	5.061468000	0.577341000
C	-5.376758000	1.936653000	4.437399000
H	-4.746881000	2.620371000	5.002578000
H	-5.963063000	2.518136000	3.733577000
H	-6.056580000	1.458392000	5.138219000
C	-2.207960000	-2.011115000	4.586849000
H	-1.143722000	-1.795817000	4.512634000
H	-2.481869000	-1.996945000	5.636791000
H	-2.371085000	-3.014678000	4.202657000
C	-7.675007000	1.410433000	-2.842603000
H	-8.750267000	1.309881000	-2.947924000
H	-7.441914000	2.462553000	-2.696514000
H	-7.209236000	1.095648000	-3.773657000
C	-8.498932000	-1.796783000	0.990285000
H	-8.983630000	-2.549555000	0.372616000
H	-7.974066000	-2.301927000	1.794458000
H	-9.278471000	-1.176991000	1.427101000
C	1.879404000	2.426908000	2.452693000
C	1.465713000	3.036777000	3.661985000
C	0.255742000	2.717275000	4.242195000
C	-0.574667000	1.790139000	3.604417000
C	-0.113753000	1.206323000	2.436699000
N	1.085620000	1.470724000	1.874366000
H	-0.052059000	3.195452000	5.168704000
H	2.117733000	3.777637000	4.115171000
H	-1.553341000	1.528210000	3.988543000
H	-0.744828000	0.498757000	1.901569000
C	3.106051000	2.892423000	1.858244000
H	3.554128000	3.725084000	2.396736000
C	3.681754000	2.522687000	0.676520000
H	4.632807000	2.966658000	0.397856000
H	3.465046000	1.588150000	0.178525000
H	3.452830000	4.210908000	-1.525043000

C	-3.550778000	-6.242101000	-2.131738000
H	-3.017042000	-6.039276000	-3.054355000
H	-2.840477000	-6.594705000	-1.390989000
H	-4.260521000	-7.040744000	-2.323719000
C	5.889218000	-0.276119000	1.368220000
C	7.098362000	-5.054081000	-0.149288000
C	7.203821000	-0.289156000	2.172232000
H	8.059813000	-0.448873000	1.524231000
H	7.335002000	0.665713000	2.672860000
H	7.195559000	-1.068488000	2.928165000
C	8.430823000	-4.582313000	-0.796140000
H	8.872535000	-3.766703000	-0.233895000
H	9.145306000	-5.399681000	-0.824538000
H	8.260763000	-4.242175000	-1.813101000
C	7.372932000	-5.530935000	1.304796000
H	8.076481000	-6.358161000	1.303063000
H	7.792665000	-4.732487000	1.907142000
H	6.454334000	-5.866863000	1.776362000
C	6.567303000	-6.263214000	-0.962406000
H	5.645876000	-6.648432000	-0.538115000
H	6.385098000	-5.991121000	-1.996821000
H	7.302248000	-7.062065000	-0.949784000
H	5.068403000	-0.030301000	2.042275000
H	5.932215000	0.531170000	0.637669000

TS2^K_{syn}, $E_{(\text{SCF Done})} = -3438.047125 \text{ a.u.}$ IF = $i189.04 \text{ cm}^{-1}$

Y	1.209757000	0.015017000	0.367693000
N	1.190935000	2.580947000	0.121050000
C	1.272169000	2.961304000	-1.302134000
H	2.327694000	3.003726000	-1.581905000
H	0.851018000	3.966366000	-1.468920000
C	0.543697000	1.974096000	-2.204637000
H	-0.522014000	1.960329000	-1.988066000
H	0.680156000	2.259716000	-3.255534000
O	1.014043000	0.629435000	-2.018052000
C	2.031859000	0.238390000	-2.938698000
H	2.318666000	-0.782693000	-2.683319000
H	2.907954000	0.888968000	-2.861539000
H	1.629330000	0.260924000	-3.958875000
O	-0.912132000	0.501112000	0.268278000
C	-1.787734000	1.481870000	0.089284000
C	-1.364827000	2.826263000	0.239066000
C	-0.001142000	3.157688000	0.785011000
H	0.105065000	4.256134000	0.790931000

H	0.063510000	2.845325000	1.835823000
C	-3.160864000	1.252658000	-0.245988000
C	-3.993854000	2.359975000	-0.417631000
H	-5.037567000	2.173940000	-0.625689000
C	-3.573188000	3.693868000	-0.327428000
C	-2.237916000	3.892435000	0.009659000
H	-1.842010000	4.895659000	0.130664000
C	-3.741084000	-0.217378000	-0.243864000
C	-4.594943000	4.853276000	-0.574185000
C	-5.744785000	4.766621000	0.468348000
H	-6.455735000	5.572517000	0.312042000
H	-5.351702000	4.849751000	1.477053000
H	-6.277894000	3.825475000	0.386803000
O	3.250266000	0.594271000	-0.114567000
C	4.069967000	1.630204000	-0.261112000
C	3.703437000	2.889488000	0.260918000
C	2.368240000	3.049726000	0.921129000
H	2.326966000	2.496293000	1.871877000
H	2.227479000	4.112515000	1.175778000
C	5.306751000	1.541277000	-0.952950000
C	6.143169000	2.658191000	-0.995550000
H	7.097779000	2.544980000	-1.498620000
C	5.816585000	3.899727000	-0.432741000
C	4.561725000	3.987813000	0.171262000
H	4.217554000	4.925220000	0.595818000
C	-5.188380000	4.728757000	-2.005638000
H	-4.401313000	4.787319000	-2.751340000
H	-5.709388000	3.786028000	-2.133475000
H	-5.894008000	5.532997000	-2.191601000
C	5.402269000	-3.684691000	-0.164095000
H	6.191200000	-3.275092000	-0.814380000
H	5.913674000	-3.958980000	0.771489000
Si	4.798314000	-5.286340000	-1.013169000
C	3.907995000	-6.462342000	0.181412000
H	4.543984000	-6.703964000	1.041491000
H	2.980049000	-6.019619000	0.557473000
H	3.655441000	-7.403851000	-0.321467000
C	6.337177000	-6.180191000	-1.690418000
H	7.037604000	-6.428199000	-0.883824000
H	6.062915000	-7.115962000	-2.191959000
H	6.872511000	-5.556279000	-2.416074000
C	3.647434000	-4.852545000	-2.461139000
H	2.747834000	-4.338934000	-2.103612000
H	4.150782000	-4.196671000	-3.182011000

H	3.330863000	-5.756182000	-2.995216000
N	1.349210000	-2.379234000	-0.048581000
C	2.016755000	-3.107029000	0.945022000
C	0.203695000	-2.912040000	-0.547692000
C	1.264244000	-4.091868000	1.670605000
C	3.383844000	-2.929518000	1.197379000
C	-0.424344000	-4.027779000	-0.041944000
H	-0.235407000	-2.368210000	-1.380662000
C	0.087208000	-4.571404000	1.162427000
H	1.710981000	-4.526196000	2.561116000
C	4.370899000	-2.571703000	0.117523000
H	-1.317589000	-4.420346000	-0.512444000
H	-0.437907000	-5.380143000	1.665516000
H	4.923988000	-1.656653000	0.369317000
H	3.816852000	-2.333800000	-0.798487000
C	-3.499061000	-0.741253000	1.205817000
C	-2.738232000	-1.859627000	1.519046000
C	-4.053293000	-0.024553000	2.272140000
C	-2.562985000	-2.264483000	2.837433000
H	-2.269138000	-2.437751000	0.738995000
C	-3.889100000	-0.432976000	3.580182000
H	-4.632996000	0.865659000	2.067628000
C	-3.141549000	-1.568085000	3.887052000
C	-3.107018000	-1.105799000	-1.357092000
C	-3.469137000	-2.452707000	-1.461834000
C	-2.322261000	-0.577526000	-2.374056000
C	-3.030063000	-3.236134000	-2.510443000
H	-4.121845000	-2.888664000	-0.717566000
C	-1.877473000	-1.366049000	-3.428461000
H	-2.077650000	0.473268000	-2.368509000
C	-2.216098000	-2.707854000	-3.511085000
C	-5.267350000	-0.248800000	-0.602225000
C	-6.243012000	-0.785318000	0.225624000
C	-5.676815000	0.192782000	-1.866593000
C	-7.573050000	-0.850094000	-0.173136000
H	-5.979766000	-1.172132000	1.198526000
C	-6.996567000	0.132477000	-2.261694000
H	-4.940976000	0.588476000	-2.553543000
C	-7.974378000	-0.390657000	-1.416166000
C	1.834790000	-0.334510000	3.955977000
C	1.411059000	-0.150100000	5.300014000
C	0.223865000	0.473746000	5.600617000
C	-0.594004000	0.895557000	4.542759000
C	-0.152738000	0.664449000	3.254258000

N	1.033689000	0.097366000	2.922424000
H	-0.076111000	0.622647000	6.634902000
H	2.065812000	-0.504557000	6.090736000
H	-1.558419000	1.363441000	4.707124000
H	-0.796132000	0.915204000	2.419149000
C	3.093366000	-0.979515000	3.752455000
H	3.506511000	-1.445059000	4.645358000
C	3.790497000	-1.105352000	2.580685000
H	3.766916000	-3.592843000	1.971723000
C	-3.928245000	6.247706000	-0.446348000
H	-3.528270000	6.402407000	0.550325000
H	-3.123367000	6.365405000	-1.164561000
H	-4.664141000	7.022817000	-0.636401000
C	5.723698000	0.230232000	-1.645083000
H	6.554518000	-0.225736000	-1.106947000
H	4.890260000	-0.461213000	-1.591007000
C	6.826561000	5.091840000	-0.521482000
H	4.796149000	-1.511763000	2.623901000
H	3.617348000	-0.461376000	1.724213000
H	-7.274598000	0.487369000	-3.245892000
H	-8.303823000	-1.276198000	0.502421000
H	-1.269476000	-0.917824000	-4.203824000
H	-3.328634000	-4.275615000	-2.559019000
H	-4.345367000	0.139367000	4.377684000
H	-1.966856000	-3.145198000	3.039915000
C	-9.442672000	-0.436794000	-1.844519000
H	-9.938997000	-1.268420000	-1.348446000
H	-9.502567000	-0.612373000	-2.916978000
C	-1.754191000	-3.571981000	-4.686639000
H	-1.586961000	-4.591142000	-4.343383000
H	-0.805670000	-3.194567000	-5.063322000
C	-2.986722000	-2.043632000	5.333332000
H	-2.022836000	-2.534560000	5.452689000
H	-3.002556000	-1.185519000	6.002449000
C	-10.193234000	0.871816000	-1.506403000
H	-11.229910000	0.805582000	-1.824010000
H	-10.174146000	1.059657000	-0.436932000
H	-9.734724000	1.718259000	-2.009090000
C	-4.106136000	-3.025424000	5.749500000
H	-3.967099000	-3.343200000	6.778923000
H	-5.080937000	-2.554139000	5.665332000
H	-4.098036000	-3.906782000	5.115111000
C	-2.783134000	-3.591668000	-5.840307000
H	-2.424884000	-4.214237000	-6.655193000

H	-3.734653000	-3.988508000	-5.499057000
H	-2.950172000	-2.589164000	-6.223105000
C	6.131267000	0.408687000	-3.125053000
H	7.017252000	1.027836000	-3.220551000
H	6.347909000	-0.558311000	-3.570096000
H	5.332885000	0.873128000	-3.696010000
C	8.156665000	4.696975000	0.179423000
H	8.608118000	3.832537000	-0.295359000
H	8.865658000	5.518218000	0.131574000
H	7.980569000	4.458646000	1.223947000
C	6.277627000	6.368927000	0.166135000
H	5.363277000	6.709257000	-0.308725000
H	6.076718000	6.192563000	1.217758000
H	7.010422000	7.166517000	0.092859000
C	7.110878000	5.426822000	-2.012732000
H	7.543256000	4.576979000	-2.529815000
H	6.193761000	5.705492000	-2.522860000
H	7.807019000	6.257101000	-2.086182000

TS2^K_{iso}, $E_{\text{(SCF Done)}} = -3438.052994$ a.u. IF = $i241.96$ cm⁻¹

Y	1.368185000	-0.300317000	-0.031200000
N	1.345275000	-2.776634000	-0.755989000
C	1.265582000	-3.680613000	0.408274000
H	2.285301000	-3.971464000	0.679202000
H	0.713289000	-4.600438000	0.160629000
C	0.595702000	-3.004409000	1.593929000
H	-0.434187000	-2.735088000	1.363091000
H	0.600422000	-3.664048000	2.471090000
O	1.259020000	-1.772890000	1.927458000
C	2.350945000	-1.912416000	2.837094000
H	2.704331000	-0.905587000	3.063464000
H	3.168534000	-2.494406000	2.398142000
H	1.999333000	-2.388737000	3.760098000
O	-0.737526000	-0.704949000	-0.255845000
C	-1.677280000	-1.618468000	-0.556408000
C	-1.215475000	-2.833320000	-1.115712000
C	0.177765000	-2.938723000	-1.669303000
H	0.276486000	-3.918272000	-2.165562000
H	0.319479000	-2.186402000	-2.459215000
C	-3.092297000	-1.446748000	-0.327356000
C	-3.884256000	-2.548107000	-0.650704000
H	-4.950663000	-2.422578000	-0.529201000
C	-3.442324000	-3.796441000	-1.108543000
C	-2.080147000	-3.901353000	-1.360125000

H	-1.661006000	-4.805533000	-1.790763000
C	-3.704882000	-0.068622000	0.131460000
C	-4.467825000	-4.953935000	-1.345019000
C	-5.502333000	-4.528207000	-2.424273000
H	-6.213128000	-5.330113000	-2.600523000
H	-5.003540000	-4.302375000	-3.361848000
H	-6.055387000	-3.648824000	-2.112164000
O	3.447957000	-0.804391000	-0.157612000
C	4.266457000	-1.849947000	-0.194762000
C	3.869151000	-3.030680000	-0.848588000
C	2.559382000	-3.057119000	-1.579566000
H	2.561863000	-2.303037000	-2.380519000
H	2.440010000	-4.037377000	-2.070389000
C	5.543660000	-1.809243000	0.422610000
C	6.347458000	-2.945339000	0.377214000
H	7.318842000	-2.900557000	0.853918000
C	5.965397000	-4.139438000	-0.259274000
C	4.710703000	-4.148349000	-0.867690000
H	4.354499000	-5.031751000	-1.387435000
C	-5.210555000	-5.268268000	-0.015940000
H	-4.505850000	-5.569604000	0.753221000
H	-5.756255000	-4.402059000	0.342376000
H	-5.919703000	-6.077301000	-0.163711000
C	2.329065000	5.536332000	0.414750000
H	1.647914000	5.870042000	1.211682000
H	3.232942000	5.186239000	0.928726000
Si	2.767487000	7.127319000	-0.551056000
C	4.202256000	6.895577000	-1.779428000
H	5.076404000	6.442331000	-1.297017000
H	3.913585000	6.261187000	-2.624810000
H	4.512900000	7.865987000	-2.185363000
C	3.290366000	8.425980000	0.736330000
H	4.166976000	8.091005000	1.303660000
H	3.548238000	9.377504000	0.256561000
H	2.483491000	8.620940000	1.452518000
C	1.248807000	7.761007000	-1.499678000
H	0.945452000	7.061554000	-2.287013000
H	0.391226000	7.906774000	-0.832509000
H	1.466699000	8.723045000	-1.978527000
N	1.381625000	1.537241000	-1.761225000
C	2.336011000	2.504410000	-2.051293000
C	0.996231000	0.714462000	-2.770273000
C	3.068275000	2.383362000	-3.279015000
C	2.627221000	3.595453000	-1.203382000

C	1. 594977000	0. 638513000	-4. 011234000
H	0. 139306000	0. 081396000	-2. 536936000
C	2. 709429000	1. 474398000	-4. 241416000
H	3. 884186000	3. 078548000	-3. 457769000
C	1. 664040000	4. 371439000	-0. 344536000
H	1. 223071000	-0. 048027000	-4. 764392000
H	3. 254748000	1. 424815000	-5. 180632000
H	1. 147417000	3. 708659000	0. 358092000
H	0. 864471000	4. 817033000	-0. 971104000
C	-3. 002685000	1. 057817000	-0. 687591000
C	-2. 564229000	2. 259689000	-0. 148739000
C	-2. 859205000	0. 884102000	-2. 069649000
C	-2. 033636000	3. 259153000	-0. 957441000
H	-2. 638210000	2. 443514000	0. 912152000
C	-2. 333312000	1. 875613000	-2. 871191000
H	-3. 185248000	-0. 041648000	-2. 524052000
C	-1. 917674000	3. 090633000	-2. 328524000
C	-3. 567759000	0. 100157000	1. 679506000
C	-4. 217305000	1. 158185000	2. 327581000
C	-2. 946347000	-0. 845917000	2. 482978000
C	-4. 244787000	1. 253628000	3. 704036000
H	-4. 744939000	1. 898434000	1. 741315000
C	-2. 975840000	-0. 752851000	3. 869913000
H	-2. 463423000	-1. 699207000	2. 030552000
C	-3. 633246000	0. 288581000	4. 504672000
C	-5. 252388000	-0. 032820000	-0. 145380000
C	-5. 834402000	0. 700187000	-1. 170667000
C	-6. 117916000	-0. 749738000	0. 690415000
C	-7. 210565000	0. 711125000	-1. 362678000
H	-5. 221642000	1. 287712000	-1. 836823000
C	-7. 484151000	-0. 742487000	0. 498737000
H	-5. 711222000	-1. 323249000	1. 511923000
C	-8. 058666000	-0. 007545000	-0. 536584000
C	2. 143811000	2. 265520000	2. 366473000
C	1. 800962000	2. 871599000	3. 598954000
C	0. 559411000	2. 668468000	4. 165853000
C	-0. 364776000	1. 859653000	3. 497190000
C	0. 040228000	1. 247922000	2. 323202000
N	1. 263624000	1. 398760000	1. 773657000
H	0. 298926000	3. 151015000	5. 104566000
H	2. 525214000	3. 528907000	4. 071082000
H	-1. 370596000	1. 703535000	3. 864907000
H	-0. 655592000	0. 614968000	1. 772692000
C	3. 382039000	2. 657755000	1. 744734000

H	3.928868000	3.412065000	2.306838000
C	3.837321000	2.341005000	0.496255000
H	4.796652000	2.734102000	0.172505000
H	3.512314000	1.464089000	-0.044050000
H	3.465095000	4.190465000	-1.563972000
C	-3.768628000	-6.251622000	-1.827020000
H	-3.269577000	-6.099451000	-2.778332000
H	-3.036965000	-6.595448000	-1.103108000
H	-4.506889000	-7.036667000	-1.957751000
C	5.962132000	-0.487771000	1.097136000
C	6.939963000	-5.364674000	-0.261895000
C	8.268052000	-4.971236000	-0.967439000
H	8.757900000	-4.151857000	-0.452548000
H	8.949863000	-5.816360000	-0.983996000
H	8.078768000	-4.665309000	-1.991844000
C	7.242355000	-5.793751000	1.201524000
H	7.913797000	-6.647173000	1.212349000
H	7.710810000	-4.988974000	1.757762000
H	6.327179000	-6.074660000	1.713958000
C	6.337950000	-6.583420000	-1.008487000
H	5.416483000	-6.915083000	-0.541212000
H	6.133522000	-6.345725000	-2.047216000
H	7.042109000	-7.409302000	-0.985316000
C	-9.571937000	-0.015465000	-0.763417000
C	-3.703482000	0.374070000	6.032000000
C	-1.386943000	4.205132000	-3.232485000
H	-8.117672000	-1.310634000	1.167816000
H	-7.622685000	1.300494000	-2.171832000
H	-2.498935000	-1.524748000	4.460430000
H	-4.773958000	2.075795000	4.168920000
H	-1.713981000	4.187829000	-0.502660000
H	-2.248607000	1.709115000	-3.937499000
H	5.991481000	0.292118000	0.336913000
H	5.183476000	-0.193983000	1.801334000
H	-10.082267000	-0.089029000	0.195101000
H	-9.874164000	0.922839000	-1.224132000
H	-3.621311000	-0.626459000	6.451633000
H	-0.739268000	3.775349000	-3.994496000
H	-0.786464000	4.893857000	-2.644013000
C	7.314323000	-0.513086000	1.835741000
H	8.131331000	-0.726427000	1.153700000
H	7.499909000	0.455844000	2.289971000
H	7.319756000	-1.261276000	2.622512000
H	-4.674225000	0.770716000	6.323783000

C	-10.022963000	-1.187641000	-1.664864000
H	-11.099941000	-1.163884000	-1.804521000
H	-9.549672000	-1.125474000	-2.640326000
H	-9.756804000	-2.140630000	-1.217250000
C	-2.597731000	1.265310000	6.641929000
H	-2.663185000	2.278556000	6.256664000
H	-2.701301000	1.304243000	7.722487000
H	-1.612812000	0.872492000	6.407945000
C	-2.525806000	4.990889000	-3.922589000
H	-2.115164000	5.770818000	-4.557409000
H	-3.130439000	4.332036000	-4.538805000
H	-3.173370000	5.456269000	-3.185246000

TS2^L_{syn}, $E_{(\text{SCF Done})} = -3555.924536 \text{ a.u.}$ IF = *i*199.31 cm⁻¹

Y	1.379342000	0.099139000	0.353616000
N	1.483746000	2.653262000	0.009587000
C	1.581351000	2.974895000	-1.426991000
H	2.636933000	2.948957000	-1.708397000
H	1.214521000	3.994268000	-1.630952000
C	0.798213000	1.996346000	-2.291651000
H	-0.266258000	2.051424000	-2.076274000
H	0.949105000	2.233826000	-3.352536000
O	1.193253000	0.635963000	-2.053608000
C	2.187521000	0.155435000	-2.957866000
H	2.421104000	-0.867974000	-2.661017000
H	3.096652000	0.761754000	-2.906412000
H	1.784689000	0.158154000	-3.978195000
O	-0.717781000	0.682102000	0.261348000
C	-1.544862000	1.696229000	0.040897000
C	-1.056636000	3.023771000	0.126780000
C	0.324394000	3.315457000	0.651625000
H	0.482171000	4.406755000	0.605779000
H	0.380801000	3.049841000	1.715651000
C	-2.928679000	1.517994000	-0.279386000
C	-3.706480000	2.654253000	-0.509376000
H	-4.757477000	2.509180000	-0.712831000
C	-3.221717000	3.969133000	-0.481790000
C	-1.878380000	4.118799000	-0.151989000
H	-1.434457000	5.106386000	-0.077810000
C	-3.573879000	0.076319000	-0.221832000
C	-4.186155000	5.163492000	-0.785861000
C	-5.338450000	5.182695000	0.257379000
H	-6.010011000	6.013194000	0.060825000
H	-4.941455000	5.295757000	1.261630000

H	-5.915983000	4.265241000	0.220553000
O	3.440315000	0.563870000	-0.163554000
C	4.311656000	1.550728000	-0.344102000
C	4.010069000	2.843711000	0.134832000
C	2.685751000	3.092585000	0.790017000
H	2.620782000	2.575841000	1.759755000
H	2.597768000	4.169442000	1.006508000
C	5.541568000	1.374814000	-1.031061000
C	6.434318000	2.445042000	-1.110675000
H	7.381535000	2.265824000	-1.608572000
C	6.172157000	3.719925000	-0.590225000
C	4.923842000	3.892710000	0.009223000
H	4.629095000	4.860328000	0.402052000
C	-4.785409000	4.999384000	-2.210882000
H	-3.996659000	4.983720000	-2.956940000
H	-5.351750000	4.078081000	-2.294433000
H	-5.451101000	5.827143000	-2.436634000
C	5.363254000	-3.831523000	-0.044819000
H	6.183713000	-3.485491000	-0.693168000
H	5.843809000	-4.099355000	0.908714000
Si	4.696233000	-5.428885000	-0.853464000
C	3.742511000	-6.529679000	0.363743000
H	4.357312000	-6.772510000	1.238752000
H	2.829276000	-6.038040000	0.714741000
H	3.456007000	-7.474279000	-0.114591000
C	6.200816000	-6.409902000	-1.485353000
H	6.882798000	-6.658861000	-0.663386000
H	5.890745000	-7.350326000	-1.956420000
H	6.769048000	-5.835777000	-2.226884000
C	3.578755000	-4.989461000	-2.325647000
H	2.697208000	-4.430356000	-1.992213000
H	4.114390000	-4.374729000	-3.059339000
H	3.230919000	-5.894484000	-2.837486000
N	1.386881000	-2.305816000	-0.018824000
C	2.006838000	-3.040113000	0.999198000
C	0.226923000	-2.796261000	-0.527036000
C	1.205150000	-3.984083000	1.725025000
C	3.378743000	-2.912326000	1.268087000
C	-0.452729000	-3.878993000	-0.016323000
H	-0.177688000	-2.246038000	-1.373170000
C	0.019045000	-4.425814000	1.202539000
H	1.619924000	-4.424439000	2.627959000
C	4.389462000	-2.655440000	0.179724000
H	-1.354017000	-4.241917000	-0.495721000

H	-0.543069000	-5.209060000	1.705927000
H	4.989624000	-1.760931000	0.393985000
H	3.853618000	-2.429919000	-0.750044000
C	-3.305952000	-0.445418000	1.224935000
C	-2.691686000	-1.654647000	1.523229000
C	-3.711859000	0.344690000	2.305121000
C	-2.526587000	-2.077693000	2.836464000
H	-2.335579000	-2.295285000	0.732944000
C	-3.553226000	-0.078815000	3.609946000
H	-4.177412000	1.302811000	2.116307000
C	-2.964453000	-1.307178000	3.903540000
C	-3.021982000	-0.857518000	-1.342706000
C	-3.491710000	-2.172738000	-1.446549000
C	-2.199822000	-0.398906000	-2.361111000
C	-3.119148000	-2.991538000	-2.491859000
H	-4.179995000	-2.552285000	-0.703486000
C	-1.822307000	-1.224853000	-3.415269000
H	-1.871452000	0.628440000	-2.361723000
C	-2.266831000	-2.533905000	-3.498413000
C	-5.115108000	0.118885000	-0.512783000
C	-6.088325000	-0.265607000	0.400503000
C	-5.553932000	0.490224000	-1.787660000
C	-7.436273000	-0.256202000	0.068304000
H	-5.807788000	-0.588307000	1.391609000
C	-6.894607000	0.503654000	-2.117283000
H	-4.827629000	0.773870000	-2.537339000
C	-7.866905000	0.132259000	-1.191588000
C	2.044441000	-0.090258000	3.940116000
C	1.678926000	0.227843000	5.276546000
C	0.538837000	0.941752000	5.559235000
C	-0.295626000	1.314536000	4.495400000
C	0.089763000	0.958602000	3.217521000
N	1.236879000	0.308766000	2.898566000
H	0.284794000	1.194073000	6.585757000
H	2.340693000	-0.097413000	6.073961000
H	-1.230567000	1.841696000	4.650509000
H	-0.566713000	1.173101000	2.382444000
C	3.249968000	-0.832359000	3.750972000
H	3.652547000	-1.272494000	4.661451000
C	3.911352000	-1.067176000	2.574421000
H	3.721030000	-3.568954000	2.066871000
C	-3.452610000	6.528538000	-0.723715000
H	-3.045203000	6.711350000	0.265158000
H	-2.643254000	6.572546000	-1.445187000

H	-4.150145000	7.328373000	-0.952123000
C	5.889544000	0.020767000	-1.676937000
H	6.699926000	-0.456107000	-1.125896000
H	5.023256000	-0.626164000	-1.594890000
C	7.242277000	4.854710000	-0.717511000
H	4.888075000	-1.538188000	2.623347000
H	3.769849000	-0.449850000	1.692927000
H	-7.192093000	0.803415000	-3.113920000
H	-8.156646000	-0.563810000	0.814604000
H	-1.183798000	-0.825683000	-4.192755000
H	-3.507506000	-4.000493000	-2.532838000
H	-3.899947000	0.553289000	4.417327000
H	-2.058046000	-3.036002000	3.013390000
C	-9.357019000	0.148904000	-1.571447000
H	-9.426119000	0.487758000	-2.604717000
C	-1.852675000	-3.432418000	-4.675638000
H	-1.181643000	-2.851531000	-5.307790000
C	-2.863915000	-1.787703000	5.361750000
H	-2.988287000	-0.913923000	6.001328000
C	-10.156018000	1.145990000	-0.696596000
H	-11.191110000	1.186479000	-1.022956000
H	-10.140284000	0.847045000	0.346728000
H	-9.734428000	2.143877000	-0.772234000
C	-4.016016000	-2.772488000	5.686888000
H	-3.974421000	-3.072963000	6.729841000
H	-4.980060000	-2.307883000	5.502400000
H	-3.943385000	-3.664018000	5.071271000
C	-3.074744000	-3.836714000	-5.536835000
H	-2.752994000	-4.418330000	-6.395765000
H	-3.773249000	-4.437062000	-4.962561000
H	-3.597546000	-2.955541000	-5.896670000
C	6.297122000	0.126164000	-3.163893000
H	7.210848000	0.698822000	-3.284877000
H	6.465365000	-0.865374000	-3.574548000
H	5.518502000	0.607195000	-3.748259000
C	-9.978498000	-1.267603000	-1.500128000
H	-11.012166000	-1.241459000	-1.832435000
H	-9.431825000	-1.957005000	-2.136576000
H	-9.957665000	-1.650757000	-0.484812000
C	-1.495215000	-2.425436000	5.698268000
H	-1.352177000	-3.356648000	5.160564000
H	-0.682654000	-1.753990000	5.440393000
H	-1.438232000	-2.639343000	6.761473000
C	-1.078667000	-4.684516000	-4.195359000

H	-1.708422000	-5.318645000	-3.579590000
H	-0.741270000	-5.266359000	-5.048065000
H	-0.209376000	-4.397156000	-3.611427000
C	8.550327000	4.415578000	-0.001569000
H	8.956466000	3.513478000	-0.446262000
H	9.300792000	5.197040000	-0.075898000
H	8.362314000	4.221977000	1.050103000
C	6.760127000	6.180905000	-0.074229000
H	5.864353000	6.551603000	-0.561594000
H	6.550776000	6.050802000	0.982477000
H	7.533024000	6.936752000	-0.173404000
C	7.543376000	5.124051000	-2.218735000
H	7.931437000	4.236116000	-2.706115000
H	6.641793000	5.432116000	-2.739537000
H	8.281328000	5.914461000	-2.318984000

TS2^L_{iso}, $E_{(\text{SCF Done})} = -3555.931288$ a.u. IF = *i*178.66 cm⁻¹

Y	1.612482000	-0.253281000	0.105251000
N	1.900264000	-2.714693000	-0.644719000
C	1.953923000	-3.640610000	0.502901000
H	3.005052000	-3.799524000	0.763262000
H	1.525448000	-4.620586000	0.241597000
C	1.211107000	-3.070245000	1.698228000
H	0.158400000	-2.908917000	1.463991000
H	1.284165000	-3.741095000	2.564065000
O	1.737512000	-1.781287000	2.052850000
C	2.874449000	-1.823439000	2.916126000
H	3.111780000	-0.791209000	3.176030000
H	3.738883000	-2.279866000	2.422529000
H	2.621276000	-2.378682000	3.827336000
O	-0.431808000	-0.896079000	-0.128137000
C	-1.250701000	-1.907270000	-0.462832000
C	-0.642737000	-3.075312000	-0.982306000
C	0.752994000	-3.031220000	-1.540930000
H	0.961712000	-4.004053000	-2.016339000
H	0.800577000	-2.287316000	-2.348459000
C	-2.686456000	-1.873389000	-0.323069000
C	-3.345915000	-3.061865000	-0.631772000
H	-4.425217000	-3.039295000	-0.579955000
C	-2.753472000	-4.275148000	-1.008081000
C	-1.380492000	-4.237911000	-1.215073000
H	-0.853378000	-5.102223000	-1.607368000
C	-3.446667000	-0.520539000	-0.054355000
C	-3.638422000	-5.545657000	-1.231074000

C	-4.652091000	-5.287163000	-2.380823000
H	-5.264199000	-6.168564000	-2.547661000
H	-4.129925000	-5.054788000	-3.303972000
H	-5.310527000	-4.458340000	-2.143886000
O	3.735973000	-0.486275000	-0.058550000
C	4.683242000	-1.415986000	-0.117283000
C	4.432498000	-2.633207000	-0.776683000
C	3.127096000	-2.822550000	-1.490064000
H	3.015999000	-2.064752000	-2.279191000
H	3.129864000	-3.804129000	-1.992743000
C	5.952306000	-1.215461000	0.485254000
C	6.896728000	-2.236580000	0.416513000
H	7.860533000	-2.070113000	0.881519000
C	6.664184000	-3.464222000	-0.228139000
C	5.412293000	-3.631108000	-0.819354000
H	5.166604000	-4.548596000	-1.344027000
C	-4.415034000	-5.871453000	0.075676000
H	-3.725239000	-6.058179000	0.893194000
H	-5.065775000	-5.051397000	0.359483000
H	-5.027761000	-6.757418000	-0.061799000
C	1.702831000	5.603668000	0.347233000
H	1.031470000	5.799317000	1.196524000
H	2.689251000	5.418107000	0.789296000
Si	1.763789000	7.250683000	-0.618444000
C	2.980252000	7.220187000	-2.080343000
H	3.990615000	6.939987000	-1.759315000
H	2.662422000	6.514951000	-2.856324000
H	3.042216000	8.213762000	-2.540731000
C	2.319769000	8.600576000	0.600332000
H	3.325205000	8.396295000	0.987510000
H	2.343447000	9.583855000	0.115826000
H	1.638885000	8.667347000	1.457091000
C	0.032845000	7.676946000	-1.274721000
H	-0.321786000	6.932867000	-1.997014000
H	-0.700458000	7.729091000	-0.461433000
H	0.040646000	8.649792000	-1.780528000
N	1.311344000	1.485108000	-1.681038000
C	2.153557000	2.538694000	-2.024179000
C	1.029752000	0.573422000	-2.650101000
C	2.942066000	2.413387000	-3.219677000
C	2.264441000	3.713502000	-1.263968000
C	1.671313000	0.484534000	-3.868637000
H	0.230593000	-0.121699000	-2.393595000
C	2.711715000	1.409438000	-4.122760000

H	3.687509000	3.177980000	-3.422616000
C	1.210017000	4.345564000	-0.397589000
H	1.386720000	-0.274535000	-4.589678000
H	3.293491000	1.350376000	-5.039341000
H	0.802522000	3.617306000	0.313135000
H	0.349423000	4.661247000	-1.025310000
C	-2.943572000	0.488702000	-1.131927000
C	-2.480170000	1.771362000	-0.862178000
C	-3.005056000	0.100461000	-2.473236000
C	-2.158759000	2.648827000	-1.890540000
H	-2.379436000	2.114683000	0.156595000
C	-2.685331000	0.973837000	-3.494064000
H	-3.340297000	-0.897620000	-2.721159000
C	-2.277027000	2.277043000	-3.223458000
C	-3.265760000	-0.034436000	1.416513000
C	-3.925089000	1.124424000	1.845812000
C	-2.639811000	-0.802585000	2.387159000
C	-3.945436000	1.494703000	3.173579000
H	-4.464692000	1.726023000	1.127072000
C	-2.668362000	-0.433277000	3.728405000
H	-2.157457000	-1.729419000	2.110846000
C	-3.319395000	0.715634000	4.147527000
C	-5.002074000	-0.711695000	-0.176954000
C	-5.787154000	-0.088263000	-1.138442000
C	-5.667173000	-1.496424000	0.770742000
C	-7.164865000	-0.256842000	-1.168703000
H	-5.333852000	0.550211000	-1.881202000
C	-7.036823000	-1.667857000	0.738549000
H	-5.098653000	-1.981795000	1.552290000
C	-7.816385000	-1.051269000	-0.237005000
C	2.375116000	2.368526000	2.495388000
C	2.188041000	2.867498000	3.807380000
C	1.205312000	2.360250000	4.630492000
C	0.365797000	1.358568000	4.133023000
C	0.589043000	0.908938000	2.843529000
N	1.577021000	1.351670000	2.037738000
H	1.077913000	2.745402000	5.638927000
H	2.839079000	3.665385000	4.151848000
H	-0.445419000	0.942132000	4.716357000
H	-0.068015000	0.150137000	2.425107000
C	3.391406000	3.001255000	1.693821000
H	3.827492000	3.877784000	2.168886000
C	3.793613000	2.704242000	0.427495000
H	4.611095000	3.267598000	-0.011824000

H	3.593744000	1.753087000	-0.045188000
H	2.999295000	4.412828000	-1.659849000
C	-2.782453000	-6.783383000	-1.606096000
H	-2.258113000	-6.629935000	-2.543459000
H	-2.053155000	-7.004524000	-0.833510000
H	-3.425340000	-7.650623000	-1.720257000
C	6.204020000	0.141721000	1.171902000
C	7.789912000	-4.551840000	-0.257720000
C	9.044934000	-3.981815000	-0.976315000
H	9.431409000	-3.110556000	-0.458631000
H	9.830692000	-4.730621000	-1.011650000
H	8.802353000	-3.693323000	-1.994522000
C	8.167098000	-4.951898000	1.196537000
H	8.944045000	-5.710563000	1.188650000
H	8.534906000	-4.098324000	1.755692000
H	7.303946000	-5.354675000	1.717873000
C	7.340884000	-5.831449000	-1.010133000
H	6.477554000	-6.285044000	-0.534361000
H	7.091807000	-5.612398000	-2.043197000
H	8.146963000	-6.558552000	-1.005961000
C	-9.341635000	-1.246285000	-0.259965000
C	-3.399478000	1.071208000	5.642452000
C	-2.006276000	3.261440000	-4.374240000
H	-7.510529000	-2.288226000	1.488439000
H	-7.732284000	0.250231000	-1.937752000
H	-2.189743000	-1.073418000	4.458542000
H	-4.480117000	2.390301000	3.459717000
H	-1.826550000	3.645860000	-1.635310000
H	-2.771871000	0.642598000	-4.520847000
H	6.136961000	0.927111000	0.419724000
H	5.394620000	0.329644000	1.877646000
H	-9.598065000	-1.907907000	0.566946000
H	-2.675425000	0.447267000	6.166312000
H	-2.172760000	2.722334000	-5.306456000
C	7.548615000	0.276970000	1.912561000
H	8.385997000	0.177342000	1.229190000
H	7.611050000	1.255371000	2.379952000
H	7.648117000	-0.475268000	2.689149000
C	-9.808495000	-1.929083000	-1.569030000
H	-10.878522000	-2.112234000	-1.536319000
H	-9.597078000	-1.303647000	-2.430566000
H	-9.302768000	-2.880331000	-1.705372000
C	-3.040985000	2.549889000	5.927184000
H	-3.780027000	3.220834000	5.502220000

H	-3.005928000	2.723451000	6.998650000
H	-2.072063000	2.802115000	5.508015000
C	-3.001798000	4.447889000	-4.337567000
H	-2.844352000	5.097184000	-5.193837000
H	-4.026811000	4.089987000	-4.364135000
H	-2.869622000	5.037530000	-3.435855000
C	-10.089502000	0.091561000	-0.039143000
H	-11.161177000	-0.079630000	0.003236000
H	-9.779591000	0.552961000	0.893741000
H	-9.888321000	0.787471000	-0.847440000
C	-4.801927000	0.734120000	6.209104000
H	-5.567215000	1.328310000	5.719131000
H	-5.034036000	-0.315457000	6.055162000
H	-4.838712000	0.940867000	7.274765000
C	-0.545298000	3.769735000	-4.381365000
H	0.147148000	2.937461000	-4.452566000
H	-0.382827000	4.425729000	-5.231584000
H	-0.320057000	4.322890000	-3.475823000

TS2^M_{syn}, $E_{(\text{SCF Done})} = -3673.80044 \text{ a.u.}$ IF = $i198.48 \text{ cm}^{-1}$

Y	1.554690000	0.150724000	0.364790000
N	1.660224000	2.694692000	-0.057032000
C	1.740152000	2.973710000	-1.503647000
H	2.792376000	2.938741000	-1.796500000
H	1.370910000	3.986683000	-1.733401000
C	0.947608000	1.969838000	-2.329538000
H	-0.114197000	2.030125000	-2.103006000
H	1.085220000	2.175850000	-3.398801000
O	1.347480000	0.617687000	-2.055983000
C	2.337380000	0.114945000	-2.952932000
H	2.578370000	-0.897761000	-2.626953000
H	3.243968000	0.726778000	-2.926844000
H	1.926933000	0.085350000	-3.969824000
O	-0.541149000	0.735299000	0.278849000
C	-1.369499000	1.744569000	0.040624000
C	-0.878062000	3.073088000	0.083215000
C	0.510496000	3.377582000	0.580492000
H	0.669069000	4.466808000	0.500525000
H	0.580764000	3.143420000	1.651023000
C	-2.757296000	1.559708000	-0.257494000
C	-3.536417000	2.690593000	-0.508617000
H	-4.589797000	2.541479000	-0.696125000
C	-3.049882000	4.005068000	-0.521923000
C	-1.702228000	4.161473000	-0.213985000

H	-1.256130000	5.149997000	-0.172477000
C	-3.403286000	0.120637000	-0.160376000
C	-4.016849000	5.192228000	-0.845521000
C	-5.156142000	5.240384000	0.210976000
H	-5.829435000	6.066125000	0.000769000
H	-4.746666000	5.379599000	1.206894000
H	-5.734766000	4.322893000	0.205660000
O	3.612099000	0.594735000	-0.184582000
C	4.482465000	1.573326000	-0.408888000
C	4.188261000	2.882442000	0.028972000
C	2.873387000	3.154580000	0.693874000
H	2.820456000	2.667156000	1.679373000
H	2.790492000	4.237669000	0.878959000
C	5.704088000	1.371376000	-1.103357000
C	6.595863000	2.437451000	-1.233477000
H	7.536645000	2.239764000	-1.736521000
C	6.340439000	3.730649000	-0.756573000
C	5.100640000	3.925563000	-0.146307000
H	4.811816000	4.906715000	0.216201000
C	-4.633827000	4.991321000	-2.258214000
H	-3.854380000	4.955040000	-3.013276000
H	-5.201912000	4.068784000	-2.310421000
H	-5.301548000	5.813631000	-2.497504000
C	5.513580000	-3.815176000	0.057268000
H	6.336345000	-3.493078000	-0.600482000
H	5.993000000	-4.061673000	1.017067000
Si	4.834153000	-5.427556000	-0.709503000
C	3.878343000	-6.494073000	0.536517000
H	4.493709000	-6.718025000	1.416177000
H	2.967001000	-5.991655000	0.877213000
H	3.588009000	-7.449014000	0.081568000
C	6.330151000	-6.433564000	-1.322250000
H	7.014056000	-6.665334000	-0.496871000
H	6.011875000	-7.383975000	-1.767086000
H	6.898855000	-5.882995000	-2.081067000
C	3.713731000	-5.017815000	-2.188089000
H	2.837132000	-4.444919000	-1.865202000
H	4.250172000	-4.425130000	-2.939122000
H	3.358065000	-5.933090000	-2.675799000
N	1.551468000	-2.262885000	0.052495000
C	2.170041000	-2.972088000	1.088743000
C	0.390792000	-2.763463000	-0.443852000
C	1.367519000	-3.897580000	1.836733000
C	3.543144000	-2.839933000	1.352314000

C	-0.289616000	-3.833302000	0.092365000
H	-0.013288000	-2.232931000	-1.302785000
C	0.181654000	-4.351454000	1.323823000
H	1.781805000	-4.316926000	2.749846000
C	4.550274000	-2.625076000	0.251099000
H	-1.191345000	-4.206616000	-0.378152000
H	-0.380511000	-5.123030000	1.844866000
H	5.159049000	-1.729619000	0.434557000
H	4.011006000	-2.423365000	-0.682069000
C	-3.119694000	-0.376671000	1.291862000
C	-2.523276000	-1.592469000	1.605286000
C	-3.499557000	0.430778000	2.364695000
C	-2.362258000	-1.998082000	2.921439000
H	-2.181942000	-2.251230000	0.823573000
C	-3.344788000	0.022165000	3.677833000
H	-3.949559000	1.395076000	2.169613000
C	-2.784151000	-1.213436000	3.990429000
C	-2.868274000	-0.836640000	-1.269339000
C	-3.346745000	-2.150802000	-1.348343000
C	-2.052905000	-0.407452000	-2.302860000
C	-2.986227000	-2.987616000	-2.381335000
H	-4.032524000	-2.514980000	-0.595421000
C	-1.686670000	-1.253997000	-3.346850000
H	-1.716737000	0.616922000	-2.328310000
C	-2.136193000	-2.562542000	-3.408811000
C	-4.948353000	0.161410000	-0.430455000
C	-5.912945000	-0.187367000	0.506350000
C	-5.407016000	0.495123000	-1.706333000
C	-7.262968000	-0.178814000	0.189961000
H	-5.623763000	-0.480773000	1.503985000
C	-6.753007000	0.507599000	-2.020662000
H	-4.692402000	0.751955000	-2.476620000
C	-7.719746000	0.172264000	-1.075396000
C	2.266986000	0.093619000	3.944423000
C	1.930199000	0.478977000	5.270787000
C	0.799805000	1.212967000	5.540639000
C	-0.056143000	1.535061000	4.476979000
C	0.302399000	1.115898000	3.210577000
N	1.442234000	0.449121000	2.900751000
H	0.569104000	1.518607000	6.558149000
H	2.606474000	0.189463000	6.069829000
H	-0.986082000	2.073249000	4.624415000
H	-0.369961000	1.290868000	2.378955000
C	3.461982000	-0.668213000	3.767609000

H	3.873999000	-1.075251000	4.689217000
C	4.104127000	-0.955964000	2.591980000
H	3.884630000	-3.475173000	2.168601000
C	-3.281332000	6.557520000	-0.828494000
H	-2.861258000	6.765677000	0.150014000
H	-2.481142000	6.581588000	-1.561044000
H	-3.980967000	7.351967000	-1.068976000
C	6.044011000	-0.006654000	-1.700978000
C	7.408446000	4.859732000	-0.940060000
H	5.076109000	-1.435939000	2.646994000
H	3.958629000	-0.369738000	1.690159000
C	6.438709000	0.041042000	-3.194326000
H	7.352343000	0.606729000	-3.345117000
H	6.601653000	-0.965829000	-3.568155000
H	5.655804000	0.500910000	-3.789888000
C	7.689058000	5.073375000	-2.454164000
H	8.425399000	5.859343000	-2.593556000
H	8.070651000	4.167945000	-2.913664000
H	6.780410000	5.362255000	-2.973681000
C	8.726236000	4.447131000	-0.226208000
H	9.475346000	5.225210000	-0.339496000
H	8.552568000	4.292501000	0.834345000
H	9.126633000	3.529178000	-0.642777000
C	6.934664000	6.208914000	-0.339795000
H	6.032039000	6.561311000	-0.828098000
H	6.740068000	6.118159000	0.723818000
H	7.705764000	6.960513000	-0.477683000
H	-7.039389000	0.780747000	-3.025097000
H	-7.968735000	-0.459231000	0.959504000
H	-1.052394000	-0.853584000	-4.123163000
H	-3.385686000	-3.992169000	-2.395427000
H	-3.682532000	0.684840000	4.460370000
H	-1.911747000	-2.963568000	3.103423000
C	-9.241562000	0.168953000	-1.380396000
C	-9.549805000	0.590695000	-2.840677000
H	-9.192886000	1.595025000	-3.043702000
H	-9.093094000	-0.090078000	-3.551429000
H	-10.622910000	0.576079000	-3.003346000
C	-9.962849000	1.163497000	-0.427362000
H	-11.028481000	1.175954000	-0.635448000
H	-9.824315000	0.882689000	0.611104000
H	-9.577181000	2.169393000	-0.563204000
C	-9.811387000	-1.260663000	-1.159099000
H	-9.317085000	-1.973150000	-1.812551000

H	-9.671370000	-1.584670000	-0.133494000
H	-10.874881000	-1.278102000	-1.377572000
C	-1.766038000	-3.538123000	-4.557554000
C	-0.792885000	-2.897598000	-5.581216000
H	-1.236774000	-2.029828000	-6.057844000
H	0.134532000	-2.596491000	-5.105060000
H	-0.554023000	-3.619942000	-6.355381000
C	-1.080974000	-4.802860000	-3.967295000
H	-1.742664000	-5.326644000	-3.286193000
H	-0.807500000	-5.486348000	-4.765388000
H	-0.179563000	-4.531832000	-3.426013000
C	-3.058104000	-3.958231000	-5.313835000
H	-3.754259000	-4.460744000	-4.650950000
H	-3.554320000	-3.088489000	-5.733797000
H	-2.813441000	-4.636688000	-6.125558000
C	-2.658991000	-1.748691000	5.442306000
C	-3.054167000	-0.683281000	6.498097000
H	-2.925666000	-1.094201000	7.494539000
H	-2.431000000	0.201055000	6.415188000
H	-4.092034000	-0.386595000	6.390366000
C	-1.197800000	-2.193623000	5.729820000
H	-0.889511000	-2.992957000	5.065472000
H	-0.512618000	-1.362063000	5.603175000
H	-1.112921000	-2.553087000	6.750808000
C	-3.604825000	-2.972369000	5.608022000
H	-4.635271000	-2.686898000	5.418964000
H	-3.338429000	-3.765219000	4.916891000
H	-3.539173000	-3.365199000	6.618283000
H	5.177288000	-0.648086000	-1.586702000
H	6.858285000	-0.464048000	-1.139229000

TS2^M_{iso}, $E_{(\text{SCF Done})} = -3673.80974 \text{ a.u.}$ IF = $i274.63 \text{ cm}^{-1}$

Y	1.746215000	-0.394031000	-0.085262000
N	1.775057000	-2.805268000	-0.984800000
C	1.662080000	-3.787413000	0.111283000
H	2.674532000	-4.086369000	0.399663000
H	1.129794000	-4.692843000	-0.219174000
C	0.939543000	-3.204113000	1.316260000
H	-0.086812000	-2.938897000	1.067623000
H	0.927171000	-3.923201000	2.145155000
O	1.564745000	-1.986699000	1.759972000
C	2.611693000	-2.165805000	2.714390000
H	2.935729000	-1.169469000	3.018210000
H	3.460154000	-2.708467000	2.283820000

H	2. 221772000	-2. 701299000	3. 588091000
O	-0. 342357000	-0. 779768000	-0. 437082000
C	-1. 262759000	-1. 685836000	-0. 814533000
C	-0. 767098000	-2. 855060000	-1. 437923000
C	0. 643554000	-2. 903301000	-1. 951029000
H	0. 770810000	-3. 839057000	-2. 519915000
H	0. 804973000	-2. 087652000	-2. 671772000
C	-2. 684690000	-1. 555837000	-0. 599253000
C	-3. 447577000	-2. 645068000	-1. 021069000
H	-4. 518376000	-2. 547122000	-0. 914358000
C	-2. 974495000	-3. 851781000	-1. 553209000
C	-1. 605594000	-3. 918074000	-1. 776794000
H	-1. 159695000	-4. 783878000	-2. 256632000
C	-3. 343972000	-0. 233794000	-0. 050148000
C	-3. 974360000	-5. 005962000	-1. 892673000
C	-4. 992553000	-4. 522267000	-2. 962973000
H	-5. 685580000	-5. 320935000	-3. 210324000
H	-4. 477685000	-4. 224037000	-3. 871167000
H	-5. 567055000	-3. 675403000	-2. 603301000
O	3. 833589000	-0. 894420000	-0. 141156000
C	4. 660085000	-1. 930632000	-0. 228323000
C	4. 299572000	-3. 051263000	-0. 998897000
C	3. 020680000	-3. 017264000	-1. 781106000
H	3. 051094000	-2. 199967000	-2. 517083000
H	2. 924029000	-3. 953839000	-2. 355177000
C	5. 906961000	-1. 943136000	0. 449577000
C	6. 718846000	-3. 069332000	0. 339956000
H	7. 666833000	-3. 065333000	0. 863504000
C	6. 373689000	-4. 203154000	-0. 416201000
C	5. 147176000	-4. 161406000	-1. 078318000
H	4. 818593000	-4. 997089000	-1. 687481000
C	-4. 739883000	-5. 424045000	-0. 605821000
H	-4. 046716000	-5. 767019000	0. 156348000
H	-5. 308245000	-4. 593742000	-0. 200768000
H	-5. 431353000	-6. 232044000	-0. 825521000
C	2. 838895000	5. 371170000	0. 834670000
H	2. 131424000	5. 675359000	1. 620577000
H	3. 690271000	4. 927567000	1. 364787000
Si	3. 421263000	7. 011805000	0. 046282000
C	4. 728819000	6. 783508000	-1. 316786000
H	5. 589734000	6. 205706000	-0. 960158000
H	4. 313857000	6. 271670000	-2. 192231000
H	5. 099844000	7. 760682000	-1. 649350000
C	4. 187779000	8. 049908000	1. 443388000

H	5.058087000	7.544851000	1.879246000
H	4.520875000	9.026465000	1.072614000
H	3.466439000	8.227890000	2.249720000
C	1.941288000	7.947372000	-0.689300000
H	1.502309000	7.404416000	-1.533754000
H	1.153412000	8.099254000	0.057609000
H	2.250245000	8.933749000	-1.055233000
N	1.840903000	1.579729000	-1.668172000
C	2.850188000	2.517498000	-1.838009000
C	1.471251000	0.849977000	-2.752070000
C	3.637109000	2.454935000	-3.033533000
C	3.147503000	3.527757000	-0.890249000
C	2.132682000	0.835161000	-3.964181000
H	0.578244000	0.241148000	-2.604639000
C	3.290780000	1.633467000	-4.077394000
H	4.488282000	3.124782000	-3.121518000
C	2.164235000	4.306849000	-0.053703000
H	1.772793000	0.221801000	-4.783568000
H	3.880973000	1.627530000	-4.990392000
H	1.555662000	3.633931000	0.559195000
H	1.441184000	4.839936000	-0.705091000
C	-2.693069000	0.982267000	-0.780211000
C	-2.407075000	2.194724000	-0.172800000
C	-2.480199000	0.904103000	-2.162538000
C	-1.984415000	3.296654000	-0.911710000
H	-2.530215000	2.316245000	0.892222000
C	-2.061123000	1.995251000	-2.892315000
H	-2.682256000	-0.024118000	-2.679434000
C	-1.829220000	3.234740000	-2.287870000
C	-3.222544000	-0.172227000	1.506661000
C	-3.938456000	0.789124000	2.232957000
C	-2.538740000	-1.123848000	2.244191000
C	-3.958645000	0.786121000	3.610464000
H	-4.521714000	1.531687000	1.705670000
C	-2.558213000	-1.127508000	3.636756000
H	-2.002811000	-1.911664000	1.737221000
C	-3.271287000	-0.181137000	4.353346000
C	-4.88859000	-0.235420000	-0.345769000
C	-5.481188000	0.510342000	-1.358624000
C	-5.745081000	-1.009930000	0.438829000
C	-6.849719000	0.479348000	-1.574403000
H	-4.879202000	1.138667000	-1.996752000
C	-7.110730000	-1.043549000	0.221524000
H	-5.337985000	-1.605952000	1.243901000

C	-7.700587000	-0.296694000	-0.794256000
C	2.380762000	2.020678000	2.488204000
C	1.946993000	2.571474000	3.717511000
C	0.635105000	2.436726000	4.124896000
C	-0.264242000	1.753702000	3.300421000
C	0.228607000	1.174221000	2.142167000
N	1.518352000	1.251487000	1.751639000
H	0.303428000	2.882811000	5.059245000
H	2.656886000	3.142678000	4.308708000
H	-1.316023000	1.665397000	3.540754000
H	-0.443388000	0.634937000	1.471227000
C	3.684579000	2.387589000	2.001971000
H	4.215515000	3.073624000	2.658902000
C	4.210122000	2.159241000	0.758028000
H	5.203675000	2.539461000	0.537011000
H	3.912589000	1.326040000	0.139119000
H	4.028477000	4.105172000	-1.167291000
C	-3.242234000	-6.255360000	-2.447810000
H	-2.724629000	-6.028681000	-3.374050000
H	-2.521207000	-6.637916000	-1.732717000
H	-3.963722000	-7.040672000	-2.650658000
C	6.290664000	-0.686965000	1.256604000
C	7.354845000	-5.421301000	-0.482242000
C	7.570760000	-0.803934000	2.106676000
H	8.443747000	-0.971508000	1.483859000
H	7.725668000	0.117162000	2.660910000
H	7.496619000	-1.619131000	2.820031000
C	8.711910000	-4.963833000	-1.086808000
H	9.172243000	-4.192771000	-0.478535000
H	9.398906000	-5.802781000	-1.146568000
H	8.568699000	-4.568027000	-2.087633000
C	7.591372000	-5.978674000	0.949725000
H	8.266854000	-6.828306000	0.916033000
H	8.028388000	-5.225774000	1.596784000
H	6.655059000	-6.306014000	1.391553000
C	6.795737000	-6.569632000	-1.361942000
H	5.856121000	-6.944265000	-0.969246000
H	6.637400000	-6.240121000	-2.383516000
H	7.503588000	-7.392473000	-1.380374000
H	5.458469000	-0.426234000	1.910172000
H	-7.712948000	-1.666561000	0.865455000
H	-7.253129000	1.083428000	-2.375182000
H	-2.014236000	-1.907831000	4.147343000
H	-4.539843000	1.542571000	4.119271000

H	-1.934721000	1.884092000	-3.960223000
H	-1.800374000	4.218326000	-0.380146000
C	-9.227053000	-0.297740000	-1.074622000
C	-10.002922000	-1.223831000	-0.102174000
H	-9.670625000	-2.252997000	-0.189788000
H	-9.878432000	-0.905549000	0.927604000
H	-11.061908000	-1.191425000	-0.338212000
C	-9.486663000	-0.793135000	-2.525386000
H	-10.552602000	-0.805447000	-2.731866000
H	-9.008677000	-0.145863000	-3.252718000
H	-9.101745000	-1.799585000	-2.659196000
C	-9.783557000	1.145414000	-0.916309000
H	-9.311097000	1.827185000	-1.615182000
H	-10.853230000	1.156919000	-1.102576000
H	-9.608590000	1.513037000	0.090281000
C	-3.363608000	-0.175333000	5.902909000
C	-2.514023000	-1.302214000	6.546063000
H	-2.855188000	-2.282159000	6.229199000
H	-1.465115000	-1.199389000	6.287781000
H	-2.601122000	-1.249972000	7.626746000
C	-4.845481000	-0.382943000	6.326419000
H	-5.476517000	0.413543000	5.946882000
H	-5.221956000	-1.327471000	5.945525000
H	-4.927850000	-0.394212000	7.409057000
C	-2.858329000	1.185515000	6.459131000
H	-1.818402000	1.344698000	6.191918000
H	-3.442211000	2.012389000	6.069757000
H	-2.936221000	1.197564000	7.541993000
C	-1.446064000	4.458700000	-3.161804000
C	-1.349598000	5.763738000	-2.330391000
H	-1.097778000	6.592546000	-2.984429000
H	-2.294573000	5.990773000	-1.847564000
H	-0.580733000	5.690343000	-1.569719000
C	-2.533206000	4.671848000	-4.254118000
H	-2.291040000	5.542903000	-4.855333000
H	-2.602859000	3.815627000	-4.915883000
H	-3.506195000	4.832113000	-3.799446000
C	-0.074583000	4.205067000	-3.846271000
H	0.701277000	4.057987000	-3.101730000
H	-0.111556000	3.324247000	-4.478274000
H	0.198564000	5.055370000	-4.463911000
H	6.403768000	0.147021000	0.564547000

TS2^{N_{syn}}, $E_{(\text{SCF Done})} = -3280.88501 \text{ a.u.}$ IF = $i191.76 \text{ cm}^{-1}$

Y	1.065462000	-0.030214000	0.326664000
N	0.957494000	2.546137000	0.103486000
C	1.016744000	2.942778000	-1.316473000
H	2.068689000	3.033351000	-1.598926000
H	0.551246000	3.929621000	-1.473650000
C	0.333003000	1.930566000	-2.225158000
H	-0.729109000	1.860286000	-2.002799000
H	0.448674000	2.232180000	-3.274103000
O	0.872514000	0.610269000	-2.052867000
C	1.912117000	0.282907000	-2.974372000
H	2.243917000	-0.727843000	-2.733329000
H	2.757377000	0.972710000	-2.884146000
H	1.513321000	0.302628000	-3.996101000
O	-1.070056000	0.393787000	0.224750000
C	-1.981418000	1.345430000	0.067929000
C	-1.604980000	2.701314000	0.236266000
C	-0.250653000	3.072285000	0.779676000
H	-0.182684000	4.173601000	0.799745000
H	-0.169992000	2.749422000	1.826288000
C	-3.348608000	1.073932000	-0.261462000
C	-4.221026000	2.154069000	-0.408396000
H	-5.259169000	1.935197000	-0.612082000
C	-3.846818000	3.500265000	-0.298603000
C	-2.516676000	3.739860000	0.031363000
H	-2.155179000	4.754208000	0.166431000
C	-3.877483000	-0.415167000	-0.285517000
C	-4.910747000	4.626900000	-0.517216000
C	-6.047967000	4.481803000	0.532649000
H	-6.788146000	5.264618000	0.395973000
H	-5.649546000	4.561508000	1.539535000
H	-6.548277000	3.523931000	0.438936000
O	3.094357000	0.622960000	-0.100681000
C	3.869382000	1.688314000	-0.271162000
C	3.453644000	2.942648000	0.224537000
C	2.121552000	3.054037000	0.899216000
H	2.108165000	2.494452000	1.846958000
H	1.944298000	4.110022000	1.159309000
C	5.102498000	1.639609000	-0.972091000
C	5.871293000	2.799357000	-1.084927000
H	6.811365000	2.714708000	-1.622259000
C	5.491774000	4.041361000	-0.557015000
C	4.252442000	4.080253000	0.083037000
H	3.869872000	5.010712000	0.489588000
C	-5.511493000	4.506061000	-1.945923000

H	-4.733273000	4.605028000	-2.696624000
H	-6.000235000	3.547925000	-2.086053000
H	-6.246415000	5.288039000	-2.112327000
C	5.360786000	-3.557051000	-0.307635000
H	6.130184000	-3.098487000	-0.948502000
H	5.885475000	-3.832544000	0.620220000
Si	4.823280000	-5.160779000	-1.196014000
C	3.975672000	-6.401190000	-0.035493000
H	4.613328000	-6.631701000	0.826422000
H	3.023548000	-6.012063000	0.339486000
H	3.773445000	-7.342360000	-0.561332000
C	6.396752000	-5.979362000	-1.888749000
H	7.102760000	-6.223363000	-1.085827000
H	6.157973000	-6.910894000	-2.415713000
H	6.911909000	-5.318153000	-2.595734000
C	3.662158000	-4.736398000	-2.638795000
H	2.739423000	-4.272221000	-2.272939000
H	4.141003000	-4.039432000	-3.337497000
H	3.387708000	-5.637200000	-3.200273000
N	1.263697000	-2.403138000	-0.167514000
C	1.949809000	-3.144727000	0.802236000
C	0.141123000	-2.955538000	-0.695769000
C	1.228865000	-4.182508000	1.483839000
C	3.309114000	-2.929087000	1.067851000
C	-0.448800000	-4.112622000	-0.238948000
H	-0.312106000	-2.394344000	-1.509282000
C	0.073612000	-4.684018000	0.947573000
H	1.684885000	-4.634315000	2.360852000
C	4.282582000	-2.497871000	0.002141000
H	-1.324348000	-4.518180000	-0.731014000
H	-0.425556000	-5.530016000	1.414497000
H	4.792479000	-1.567252000	0.282646000
H	3.721741000	-2.255672000	-0.908777000
C	-3.597173000	-0.965737000	1.147180000
C	-2.802975000	-2.071052000	1.421508000
C	-4.153646000	-0.290409000	2.238925000
C	-2.596847000	-2.503344000	2.726650000
H	-2.331308000	-2.617751000	0.620649000
C	-3.959627000	-0.726432000	3.533939000
H	-4.759585000	0.588806000	2.065219000
C	-3.178782000	-1.849127000	3.801475000
C	-3.228591000	-1.253855000	-1.428403000
C	-3.553824000	-2.608259000	-1.567118000
C	-2.471321000	-0.676218000	-2.437695000

C	-3.104506000	-3.349116000	-2.640504000
H	-4.187765000	-3.082134000	-0.829804000
C	-2.014404000	-1.422719000	-3.518623000
H	-2.259255000	0.381122000	-2.407545000
C	-2.316636000	-2.769438000	-3.635572000
C	-5.407028000	-0.491093000	-0.623169000
C	-6.353585000	-1.066594000	0.209373000
C	-5.847987000	-0.043968000	-1.876916000
C	-7.688444000	-1.166257000	-0.172151000
H	-6.066592000	-1.457502000	1.173838000
C	-7.169025000	-0.138627000	-2.254444000
H	-5.133986000	0.384406000	-2.567302000
C	-8.120306000	-0.701994000	-1.401046000
C	1.684334000	-0.463713000	3.904931000
C	1.250478000	-0.321709000	5.251115000
C	0.056458000	0.283570000	5.561921000
C	-0.759234000	0.728024000	4.511480000
C	-0.309266000	0.535010000	3.219876000
N	0.883925000	-0.012079000	2.879101000
H	-0.250477000	0.401166000	6.598200000
H	1.903997000	-0.692031000	6.035561000
H	-1.728565000	1.182862000	4.683331000
H	-0.951996000	0.800130000	2.388714000
C	2.951885000	-1.086778000	3.691163000
H	3.363507000	-1.577376000	4.571277000
C	3.662096000	-1.158396000	2.521895000
H	3.713163000	-3.613720000	1.812368000
C	-4.292426000	6.041587000	-0.370253000
H	-3.889723000	6.193142000	0.625806000
H	-3.498286000	6.199961000	-1.092590000
H	-5.056704000	6.793388000	-0.540935000
C	5.612263000	0.342498000	-1.609826000
H	6.277090000	-0.192646000	-0.935627000
H	4.788848000	-0.317601000	-1.856148000
H	6.167179000	0.560286000	-2.517916000
C	6.428324000	5.284143000	-0.721004000
H	4.674775000	-1.547577000	2.561520000
H	3.487255000	-0.480735000	1.692186000
H	-7.472821000	0.222778000	-3.228621000
H	-8.396219000	-1.621091000	0.508908000
H	-1.430519000	-0.934858000	-4.288409000
H	-3.377346000	-4.393882000	-2.718031000
H	-4.419343000	-0.186738000	4.351853000
H	-1.975459000	-3.372957000	2.898492000

C	-9.582413000	-0.802436000	-1.826997000
H	-10.171381000	-1.309510000	-1.069731000
H	-10.007493000	0.186515000	-1.984021000
H	-9.675994000	-1.353712000	-2.759688000
C	-1.810992000	-3.601093000	-4.811093000
H	-0.993281000	-4.248451000	-4.499580000
H	-2.601484000	-4.233341000	-5.206316000
H	-1.449171000	-2.961973000	-5.610158000
C	-2.987809000	-2.352771000	5.229708000
H	-2.027131000	-2.846532000	5.341025000
H	-3.040598000	-1.533936000	5.940842000
H	-3.763826000	-3.070446000	5.490544000
C	7.800358000	4.990466000	-0.051973000
H	8.285178000	4.135889000	-0.511481000
H	8.459260000	5.847910000	-0.152149000
H	7.671323000	4.780992000	1.005532000
C	5.828867000	6.552658000	-0.060268000
H	4.881966000	6.823361000	-0.515743000
H	5.671631000	6.403866000	1.002995000
H	6.511983000	7.386989000	-0.185748000
C	6.645653000	5.579079000	-2.231825000
H	7.290629000	6.443657000	-2.357787000
H	7.109293000	4.736120000	-2.732871000
H	5.698464000	5.787068000	-2.720269000

TS2^N_{iso}, $E_{\text{(SCF Done)}} = -3280.889082$ a.u. IF = $i222.12$ cm⁻¹

Y	1.235442000	-0.247482000	0.083687000
N	1.221762000	-2.735250000	-0.621950000
C	1.112922000	-3.630238000	0.546931000
H	2.125096000	-3.923358000	0.842687000
H	0.562601000	-4.549649000	0.293358000
C	0.420439000	-2.942404000	1.712198000
H	-0.602025000	-2.666802000	1.456103000
H	0.400223000	-3.596240000	2.593584000
O	1.085600000	-1.714023000	2.052114000
C	2.164818000	-1.858272000	2.976130000
H	2.521367000	-0.852963000	3.204167000
H	2.984528000	-2.446150000	2.549281000
H	1.798420000	-2.330432000	3.895552000
O	-0.863941000	-0.646147000	-0.178181000
C	-1.800225000	-1.550765000	-0.514626000
C	-1.333130000	-2.775563000	-1.047728000
C	0.075106000	-2.906123000	-1.559226000
H	0.176593000	-3.897124000	-2.031791000

H	0.244643000	-2.173914000	-2.361866000
C	-3.220831000	-1.356441000	-0.349020000
C	-4.016495000	-2.448078000	-0.693543000
H	-5.085090000	-2.304744000	-0.618179000
C	-3.573892000	-3.706920000	-1.121141000
C	-2.204222000	-3.832919000	-1.316652000
H	-1.781894000	-4.746767000	-1.723053000
C	-3.823831000	0.039385000	0.063195000
C	-4.605218000	-4.852090000	-1.390218000
C	-5.586152000	-4.422539000	-2.516947000
H	-6.300507000	-5.215905000	-2.715983000
H	-5.044375000	-4.213334000	-3.434312000
H	-6.139014000	-3.532209000	-2.237209000
O	3.312624000	-0.758921000	0.001317000
C	4.129090000	-1.805535000	-0.007639000
C	3.747228000	-2.994764000	-0.656786000
C	2.453169000	-3.028723000	-1.415671000
H	2.474736000	-2.284655000	-2.225399000
H	2.342096000	-4.015047000	-1.896208000
C	5.389106000	-1.762258000	0.637219000
C	6.197743000	-2.896810000	0.623641000
H	7.156525000	-2.830168000	1.129081000
C	5.833658000	-4.097186000	-0.009448000
C	4.590969000	-4.111008000	-0.645226000
H	4.246897000	-5.000152000	-1.163509000
C	-5.408761000	-5.142111000	-0.091342000
H	-4.742173000	-5.445644000	0.710250000
H	-5.956475000	-4.264545000	0.234821000
H	-6.122810000	-5.942346000	-0.261684000
C	2.201456000	5.580936000	0.345793000
H	1.514428000	5.929417000	1.131373000
H	3.103611000	5.246435000	0.872784000
Si	2.637318000	7.152016000	-0.652477000
C	4.060192000	6.893737000	-1.889144000
H	4.939547000	6.451487000	-1.405952000
H	3.763779000	6.241367000	-2.717989000
H	4.366058000	7.855538000	-2.318550000
C	3.174989000	8.472275000	0.606641000
H	4.057413000	8.146286000	1.170225000
H	3.428345000	9.415243000	0.107957000
H	2.376024000	8.680355000	1.328018000
C	1.111472000	7.771636000	-1.598600000
H	0.792287000	7.052873000	-2.361960000
H	0.264116000	7.942378000	-0.924320000

H	1. 330090000	8. 718410000	-2. 106622000
N	1. 278210000	1. 523909000	-1. 707116000
C	2. 243730000	2. 473822000	-2. 021366000
C	0. 901110000	0. 666941000	-2. 691404000
C	2. 999962000	2. 294360000	-3. 228698000
C	2. 517815000	3. 600687000	-1. 221163000
C	1. 520697000	0. 536532000	-3. 917088000
H	0. 033269000	0. 053404000	-2. 448686000
C	2. 649836000	1. 350472000	-4. 159227000
H	3. 826260000	2. 974044000	-3. 419225000
C	1. 546202000	4. 396293000	-0. 391241000
H	1. 153197000	-0. 173409000	-4. 650449000
H	3. 212407000	1. 256555000	-5. 084817000
H	1. 024721000	3. 749097000	0. 322871000
H	0. 752916000	4. 824199000	-1. 038809000
C	-3. 084237000	1. 132521000	-0. 767744000
C	-2. 606095000	2. 325088000	-0. 239936000
C	-2. 937009000	0. 935885000	-2. 145266000
C	-2. 033920000	3. 293335000	-1. 056148000
H	-2. 681680000	2. 525517000	0. 817791000
C	-2. 367316000	1. 897110000	-2. 955388000
H	-3. 293674000	0. 016992000	-2. 590714000
C	-1. 911343000	3. 101918000	-2. 424452000
C	-3. 707021000	0. 250117000	1. 606559000
C	-4. 332540000	1. 349788000	2. 209491000
C	-3. 115476000	-0. 680348000	2. 447490000
C	-4. 348656000	1. 508225000	3. 578715000
H	-4. 838816000	2. 078823000	1. 591187000
C	-3. 135619000	-0. 525185000	3. 830091000
H	-2. 656398000	-1. 564690000	2. 031373000
C	-3. 750815000	0. 566374000	4. 418300000
C	-5. 364993000	0. 091994000	-0. 237170000
C	-5. 924238000	0. 826342000	-1. 271610000
C	-6. 249880000	-0. 610313000	0. 593396000
C	-7. 299472000	0. 853013000	-1. 481285000
H	-5. 296242000	1. 402582000	-1. 933562000
C	-7. 611716000	-0. 587711000	0. 385165000
H	-5. 858579000	-1. 184377000	1. 422119000
C	-8. 164762000	0. 148403000	-0. 663898000
C	2. 075774000	2. 338200000	2. 447336000
C	1. 786173000	2. 949589000	3. 691386000
C	0. 599866000	2. 697639000	4. 348119000
C	-0. 329260000	1. 836383000	3. 755367000
C	0. 015166000	1. 241767000	2. 553750000

N	1. 187773000	1. 440049000	1. 914504000
H	0. 385408000	3. 178035000	5. 299414000
H	2. 513316000	3. 640355000	4. 107919000
H	-1. 295039000	1. 631717000	4. 200224000
H	-0. 692054000	0. 577680000	2. 059467000
C	3. 280553000	2. 747589000	1. 771980000
H	3. 819996000	3. 533409000	2. 296893000
C	3. 733327000	2. 389180000	0. 535615000
H	4. 679684000	2. 791925000	0. 186965000
H	3. 418631000	1. 487970000	0. 029665000
H	3. 359067000	4. 184365000	-1. 591956000
C	-3. 905352000	-6. 164583000	-1. 829251000
H	-3. 364753000	-6. 029704000	-2. 760246000
H	-3. 209715000	-6. 510879000	-1. 071774000
H	-4. 648822000	-6. 940497000	-1. 982971000
C	5. 838687000	-0. 470336000	1. 325048000
C	6. 808144000	-5. 321743000	0. 020963000
C	8. 152161000	-4. 932627000	-0. 656182000
H	8. 628300000	-4. 107952000	-0. 136873000
H	8. 835233000	-5. 776861000	-0. 648978000
H	7. 987003000	-4. 635953000	-1. 687457000
C	7. 076181000	-5. 737694000	1. 494801000
H	7. 748309000	-6. 589958000	1. 529022000
H	7. 530181000	-4. 927202000	2. 054748000
H	6. 149464000	-6. 015477000	1. 987833000
C	6. 224402000	-6. 546980000	-0. 729419000
H	5. 292726000	-6. 875814000	-0. 280750000
H	6. 043664000	-6. 317711000	-1. 774426000
H	6. 928528000	-7. 371935000	-0. 683484000
C	-9. 674559000	0. 171051000	-0. 885883000
C	-3. 806601000	0. 730863000	5. 935020000
C	-1. 279397000	4. 161082000	-3. 322917000
H	-8. 261285000	-1. 145856000	1. 047272000
H	-7. 693603000	1. 441348000	-2. 299915000
H	-2. 672589000	-1. 280103000	4. 452547000
H	-4. 845612000	2. 367975000	4. 009912000
H	-1. 688540000	4. 217333000	-0. 611451000
H	-2. 282513000	1. 714992000	-4. 019080000
H	6. 783741000	-0. 618091000	1. 838071000
H	5. 964731000	0. 329357000	0. 599238000
H	5. 101457000	-0. 136350000	2. 051990000
H	-10. 051767000	-0. 831225000	-1. 076158000
H	-9. 930878000	0. 798327000	-1. 733381000
H	-10. 188165000	0. 555868000	-0. 007816000

H	-3.134628000	0.033825000	6.425381000
H	-4.813390000	0.546104000	6.304368000
H	-3.529036000	1.740403000	6.226900000
H	-0.216640000	3.965366000	-3.452466000
H	-1.742423000	4.160025000	-4.305458000
H	-1.388280000	5.150582000	-2.889969000

TS2⁰_{syn}, $E_{\text{(SCF Done)}} = -3398.756246$ a.u. IF = $i192.80$ cm⁻¹

Y	1.305244000	0.020898000	0.336743000
N	1.266064000	2.597090000	0.108886000
C	1.323015000	2.990347000	-1.312148000
H	2.374270000	3.053570000	-1.604294000
H	0.881761000	3.988706000	-1.466325000
C	0.604283000	1.995490000	-2.212956000
H	-0.457517000	1.955606000	-1.981675000
H	0.719786000	2.291401000	-3.263522000
O	1.107923000	0.661026000	-2.041687000
C	2.128365000	0.300644000	-2.972164000
H	2.432502000	-0.718778000	-2.731016000
H	2.994299000	0.965463000	-2.892089000
H	1.720503000	0.329170000	-3.990092000
O	-0.819941000	0.500166000	0.251018000
C	-1.706105000	1.476611000	0.103164000
C	-1.290629000	2.821857000	0.265954000
C	0.078791000	3.157093000	0.794860000
H	0.176636000	4.256208000	0.810939000
H	0.161096000	2.835140000	1.841596000
C	-3.083869000	1.242602000	-0.210847000
C	-3.928043000	2.346189000	-0.347896000
H	-4.974063000	2.155705000	-0.539353000
C	-3.515926000	3.681682000	-0.243176000
C	-2.175936000	3.884882000	0.070824000
H	-1.785222000	4.889016000	0.200838000
C	-3.653179000	-0.231726000	-0.228935000
C	-4.551145000	4.836970000	-0.449724000
C	-5.679376000	4.723217000	0.613617000
H	-6.399449000	5.525961000	0.485371000
H	-5.266988000	4.792147000	1.615664000
H	-6.206758000	3.779365000	0.526308000
O	3.348095000	0.617077000	-0.109658000
C	4.150175000	1.660534000	-0.289551000
C	3.772979000	2.926619000	0.207228000
C	2.450361000	3.075088000	0.893245000
H	2.430216000	2.518161000	1.842388000

H	2. 303878000	4. 136041000	1. 152322000
C	5. 375215000	1. 577401000	-1. 001422000
C	6. 174147000	2. 715661000	-1. 123128000
H	7. 106645000	2. 604648000	-1. 668784000
C	5. 833326000	3. 968316000	-0. 593973000
C	4. 601182000	4. 041818000	0. 056845000
H	4. 247675000	4. 982951000	0. 465177000
C	-5. 171903000	4. 732427000	-1. 871142000
H	-4. 400246000	4. 810039000	-2. 631072000
H	-5. 688194000	3. 787946000	-2. 005036000
H	-5. 887152000	5. 534141000	-2. 029162000
C	5. 506469000	-3. 612156000	-0. 313115000
H	6. 284050000	-3. 173529000	-0. 958057000
H	6. 027722000	-3. 896203000	0. 614131000
Si	4. 930211000	-5. 206431000	-1. 194668000
C	4. 059785000	-6. 423230000	-0. 026227000
H	4. 696208000	-6. 666370000	0. 833101000
H	3. 119680000	-6. 009168000	0. 352220000
H	3. 831663000	-7. 360801000	-0. 547840000
C	6. 483455000	-6. 060386000	-1. 890235000
H	7. 186856000	-6. 316647000	-1. 088838000
H	6. 223904000	-6. 988213000	-2. 413891000
H	7. 009911000	-5. 411737000	-2. 600540000
C	3. 772839000	-4. 761958000	-2. 634269000
H	2. 861636000	-4. 276507000	-2. 266925000
H	4. 263850000	-4. 078223000	-3. 337565000
H	3. 476701000	-5. 658790000	-3. 191035000
N	1. 435995000	-2. 357069000	-0. 156117000
C	2. 109224000	-3. 114149000	0. 810465000
C	0. 295653000	-2. 880735000	-0. 675400000
C	1. 367004000	-4. 132705000	1. 498015000
C	3. 475250000	-2. 931928000	1. 068120000
C	-0. 321273000	-4. 021099000	-0. 212139000
H	-0. 148584000	-2. 309472000	-1. 486912000
C	0. 195062000	-4. 604660000	0. 971031000
H	1. 817717000	-4. 595598000	2. 371972000
C	4. 453496000	-2. 527694000	-0. 003930000
H	-1. 210749000	-4. 404111000	-0. 697250000
H	-0. 322154000	-5. 437087000	1. 442671000
H	4. 984944000	-1. 607049000	0. 269423000
H	3. 894289000	-2. 277713000	-0. 913744000
C	-3. 373367000	-0. 789209000	1. 201210000
C	-2. 603809000	-1. 913662000	1. 468242000
C	-3. 903129000	-0. 100485000	2. 297894000

C	-2.396465000	-2.350782000	2.771575000
H	-2.153267000	-2.471567000	0.662948000
C	-3.707867000	-0.541525000	3.591060000
H	-4.488953000	0.793278000	2.129458000
C	-2.951445000	-1.682229000	3.851693000
C	-3.039269000	-1.087913000	-1.378257000
C	-3.399796000	-2.432762000	-1.511734000
C	-2.276469000	-0.530413000	-2.396136000
C	-2.980220000	-3.186324000	-2.589760000
H	-4.036142000	-2.890563000	-0.766392000
C	-1.850719000	-1.288964000	-3.479943000
H	-2.034956000	0.520643000	-2.367470000
C	-2.187735000	-2.628962000	-3.591921000
C	-5.187640000	-0.266363000	-0.551148000
C	-6.140576000	-0.821834000	0.290536000
C	-5.629818000	0.194739000	-1.797481000
C	-7.479584000	-0.886505000	-0.077092000
H	-5.852294000	-1.223959000	1.250003000
C	-6.958435000	0.134605000	-2.161612000
H	-4.912755000	0.605967000	-2.495076000
C	-7.913084000	-0.407837000	-1.301888000
C	1.936557000	-0.421022000	3.912092000
C	1.516781000	-0.263214000	5.261012000
C	0.342179000	0.375581000	5.578609000
C	-0.468793000	0.839030000	4.532741000
C	-0.034125000	0.629534000	3.238499000
N	1.141058000	0.048904000	2.890622000
H	0.046346000	0.504848000	6.616726000
H	2.165830000	-0.648780000	6.041807000
H	-1.423924000	1.320934000	4.710222000
H	-0.675606000	0.909668000	2.411365000
C	3.185380000	-1.078010000	3.690645000
H	3.590652000	-1.577532000	4.568675000
C	3.884514000	-1.170215000	2.516035000
H	3.865727000	-3.625004000	1.812042000
C	-3.892682000	6.234250000	-0.310786000
H	-3.474166000	6.374873000	0.680345000
H	-3.103151000	6.370744000	-1.042577000
H	-4.638089000	7.006653000	-0.472723000
C	5.843919000	0.266034000	-1.641585000
H	6.500314000	-0.285862000	-0.972658000
H	5.000759000	-0.371992000	-1.879155000
H	6.396036000	0.467447000	-2.555148000
C	6.801847000	5.184877000	-0.768457000

H	4.887210000	-1.585056000	2.548693000
H	3.721402000	-0.488798000	1.686980000
H	-7.261831000	0.504995000	-3.132515000
H	-8.191758000	-1.327811000	0.608494000
H	-1.259212000	-0.818284000	-4.254779000
H	-3.277393000	-4.224939000	-2.660448000
H	-4.146470000	0.009395000	4.413170000
H	-1.794589000	-3.235169000	2.937823000
C	-9.391144000	-0.453819000	-1.695225000
H	-9.871171000	-1.297183000	-1.202937000
H	-9.476352000	-0.609652000	-2.769016000
C	-1.747754000	-3.459663000	-4.799539000
H	-1.572763000	-4.487624000	-4.487851000
H	-0.807160000	-3.070440000	-5.184016000
C	-2.762217000	-2.194048000	5.281394000
H	-1.793284000	-2.682125000	5.366843000
H	-2.767933000	-1.353603000	5.972689000
C	-10.139565000	0.844243000	-1.314382000
H	-11.183364000	0.778459000	-1.607837000
H	-10.095247000	1.012159000	-0.242348000
H	-9.697587000	1.702357000	-1.812064000
C	-3.866859000	-3.192969000	5.696293000
H	-3.703412000	-3.536513000	6.713784000
H	-4.845825000	-2.725511000	5.645844000
H	-3.868018000	-4.057525000	5.039139000
C	-2.798892000	-3.449218000	-5.933151000
H	-2.455875000	-4.048484000	-6.771718000
H	-3.743168000	-3.856859000	-5.584592000
H	-2.974428000	-2.436806000	-6.284802000
C	8.171426000	4.854856000	-0.111440000
H	8.628564000	3.986730000	-0.573916000
H	8.852509000	5.693873000	-0.219033000
H	8.046401000	4.650469000	0.947540000
C	6.243211000	6.470171000	-0.104388000
H	5.299957000	6.765981000	-0.551744000
H	6.091607000	6.327166000	0.960486000
H	6.947656000	7.285389000	-0.237361000
C	7.013357000	5.471677000	-2.281674000
H	7.680497000	6.318159000	-2.414915000
H	7.449250000	4.615682000	-2.785522000
H	6.067780000	5.704744000	-2.761849000

TS2⁰_{iso}, $E_{\text{(SCF Done)}} = -3398.763827$ a.u. IF = $i210.36$ cm⁻¹

Y	1.484731000	-0.294660000	0.074040000
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N	1.499983000	-2.760692000	-0.708251000
C	1.402737000	-3.692427000	0.432346000
H	2.418564000	-3.982337000	0.718535000
H	0.863123000	-4.610113000	0.151124000
C	0.703182000	-3.048854000	1.618449000
H	-0.322458000	-2.776380000	1.371294000
H	0.690688000	-3.729800000	2.479227000
O	1.354970000	-1.824302000	1.996205000
C	2.439471000	-1.985426000	2.911281000
H	2.782091000	-0.983712000	3.173771000
H	3.266332000	-2.545276000	2.461341000
H	2.083135000	-2.495180000	3.814396000
O	-0.611879000	-0.707110000	-0.202859000
C	-1.536415000	-1.613184000	-0.566768000
C	-1.054376000	-2.817628000	-1.131613000
C	0.354140000	-2.914557000	-1.649036000
H	0.466649000	-3.888140000	-2.154197000
H	0.513131000	-2.153636000	-2.426890000
C	-2.959831000	-1.438215000	-0.403434000
C	-3.742026000	-2.530615000	-0.774764000
H	-4.812464000	-2.400526000	-0.701095000
C	-3.283514000	-3.774238000	-1.229761000
C	-1.912393000	-3.878561000	-1.427582000
H	-1.478809000	-4.776432000	-1.857117000
C	-3.577042000	-0.054348000	0.026822000
C	-4.300642000	-4.925072000	-1.527178000
C	-5.283275000	-4.482472000	-2.647360000
H	-5.987675000	-5.279573000	-2.866010000
H	-4.741313000	-4.246871000	-3.558193000
H	-5.847388000	-3.605016000	-2.349949000
O	3.567950000	-0.778325000	-0.030397000
C	4.396595000	-1.814716000	-0.070208000
C	4.027666000	-2.988941000	-0.753369000
C	2.733469000	-3.014871000	-1.511959000
H	2.745068000	-2.245770000	-2.298076000
H	2.633444000	-3.986986000	-2.022979000
C	5.656458000	-1.776393000	0.575295000
C	6.477391000	-2.901262000	0.528751000
H	7.435605000	-2.838745000	1.035793000
C	6.126131000	-4.086876000	-0.138422000
C	4.883369000	-4.095847000	-0.774118000
H	4.548590000	-4.973328000	-1.317753000
C	-5.104566000	-5.252703000	-0.237507000
H	-4.436855000	-5.566173000	0.559311000

H	-5.663182000	-4.388785000	0.106133000
H	-5.808934000	-6.057074000	-0.427560000
C	2.411055000	5.535696000	0.546785000
H	1.762247000	5.824332000	1.387219000
H	3.348929000	5.195313000	1.002888000
Si	2.744067000	7.168605000	-0.389038000
C	3.946783000	6.979469000	-1.850225000
H	4.897587000	6.533202000	-1.535292000
H	3.524176000	6.354852000	-2.645030000
H	4.170049000	7.961865000	-2.284067000
C	3.505103000	8.384903000	0.858938000
H	4.461794000	8.010906000	1.242904000
H	3.691358000	9.360860000	0.395407000
H	2.840380000	8.544110000	1.716192000
C	1.105451000	7.878212000	-1.037097000
H	0.647300000	7.219965000	-1.784105000
H	0.382331000	8.015160000	-0.224609000
H	1.264353000	8.854307000	-1.510671000
N	1.489645000	1.547179000	-1.644004000
C	2.437965000	2.521920000	-1.935225000
C	1.115043000	0.719147000	-2.654222000
C	3.184718000	2.394428000	-3.155637000
C	2.706873000	3.624529000	-1.101775000
C	1.724506000	0.639358000	-3.889227000
H	0.257668000	0.085961000	-2.424851000
C	2.839274000	1.477948000	-4.114359000
H	3.999147000	3.092348000	-3.330739000
C	1.744888000	4.376398000	-0.222493000
H	1.359761000	-0.050459000	-4.642903000
H	3.394121000	1.423678000	-5.047768000
H	1.241517000	3.697569000	0.475205000
H	0.934916000	4.822474000	-0.836996000
C	-2.860972000	1.048858000	-0.811276000
C	-2.366927000	2.236410000	-0.286663000
C	-2.746044000	0.860367000	-2.192973000
C	-1.812116000	3.208508000	-1.110692000
H	-2.413823000	2.428321000	0.774433000
C	-2.193607000	1.825439000	-3.010240000
H	-3.112288000	-0.056399000	-2.634924000
C	-1.720774000	3.024866000	-2.482588000
C	-3.448500000	0.148536000	1.569891000
C	-4.062561000	1.248163000	2.181577000
C	-2.866774000	-0.796919000	2.403216000
C	-4.078676000	1.393880000	3.553504000

H	-4.561310000	1.987835000	1.569841000
C	-2.888839000	-0.655049000	3.785882000
H	-2.416253000	-1.681724000	1.978432000
C	-3.493342000	0.438712000	4.384172000
C	-5.123028000	-0.019215000	-0.251220000
C	-5.709674000	0.737657000	-1.255986000
C	-5.983638000	-0.754481000	0.573564000
C	-7.086820000	0.750970000	-1.441685000
H	-5.099887000	1.341823000	-1.910045000
C	-7.350545000	-0.744955000	0.387917000
H	-5.571416000	-1.343899000	1.381109000
C	-7.930157000	0.012035000	-0.628782000
C	2.328506000	2.213976000	2.523676000
C	2.047709000	2.776171000	3.792460000
C	0.870019000	2.491435000	4.451384000
C	-0.058589000	1.646087000	3.835919000
C	0.278004000	1.098755000	2.609761000
N	1.442305000	1.329164000	1.966535000
H	0.661820000	2.934347000	5.422036000
H	2.774397000	3.456060000	4.227217000
H	-1.018586000	1.418419000	4.281770000
H	-0.429544000	0.447118000	2.099630000
C	3.523275000	2.659572000	1.852567000
H	4.060257000	3.430660000	2.401257000
C	3.967151000	2.351612000	0.600708000
H	4.904270000	2.778447000	0.255824000
H	3.650656000	1.471444000	0.060386000
H	3.535589000	4.231943000	-1.462337000
C	-3.584233000	-6.219497000	-1.992398000
H	-3.043541000	-6.058493000	-2.919171000
H	-2.885877000	-6.573321000	-1.240918000
H	-4.317995000	-7.000868000	-2.164097000
C	6.092672000	-0.500538000	1.300628000
C	7.113638000	-5.301319000	-0.142961000
C	8.453243000	-4.878775000	-0.808703000
H	8.920695000	-4.064185000	-0.266106000
H	9.145276000	-5.715541000	-0.825506000
H	8.284652000	-4.554645000	-1.831119000
C	7.386501000	-5.756243000	1.318431000
H	8.067639000	-6.601958000	1.328359000
H	7.832041000	-4.957270000	1.901263000
H	6.462926000	-6.057788000	1.803335000
C	6.542726000	-6.510815000	-0.927954000
H	5.614749000	-6.862202000	-0.488815000

H	6.359211000	-6.253788000	-1.965994000
H	7.255602000	-7.329205000	-0.905567000
C	-9.444318000	0.006786000	-0.849759000
C	-3.559203000	0.575837000	5.907306000
C	-1.149493000	4.110403000	-3.396971000
H	-7.980862000	-1.328045000	1.047100000
H	-7.503463000	1.358439000	-2.234989000
H	-2.434911000	-1.420394000	4.402522000
H	-4.566082000	2.255752000	3.991349000
H	-1.449634000	4.126761000	-0.667742000
H	-2.129657000	1.647449000	-4.076119000
H	7.039694000	-0.653186000	1.808561000
H	6.209522000	0.321516000	0.598679000
H	5.352536000	-0.196089000	2.037504000
H	-9.950708000	-0.091941000	0.108581000
H	-9.750211000	0.955782000	-1.285496000
H	-2.705057000	0.071886000	6.355335000
H	-3.499054000	1.627749000	6.180563000
H	-0.647306000	3.643010000	-4.241575000
H	-0.405304000	4.687760000	-2.853673000
C	-9.896723000	-1.143166000	-1.778730000
H	-10.974300000	-1.118101000	-1.913473000
H	-9.427490000	-1.055403000	-2.754185000
H	-9.626901000	-2.106619000	-1.356422000
C	-4.859374000	-0.021184000	6.492879000
H	-4.934285000	-1.079310000	6.260241000
H	-4.874868000	0.094392000	7.572867000
H	-5.730481000	0.480445000	6.082029000
C	-2.244419000	5.065439000	-3.925924000
H	-1.806634000	5.821065000	-4.571930000
H	-2.989670000	4.518550000	-4.496109000
H	-2.746113000	5.567704000	-3.103981000

TS2^P_{iso}, $E_{(\text{SCF Done})} = -2465.424363 \text{ a.u.}$ IF = *i*88.37 cm⁻¹

Y	0.474447000	0.655818000	0.468772000
N	1.375040000	-1.618991000	-0.582668000
C	1.782708000	-2.615709000	0.426734000
H	2.851379000	-2.480338000	0.618911000
H	1.644939000	-3.641699000	0.049023000
C	1.017480000	-2.449862000	1.727061000
H	-0.049725000	-2.626755000	1.584942000
H	1.387939000	-3.157158000	2.482006000
O	1.140741000	-1.114343000	2.219699000
C	2.271324000	-0.903885000	3.059167000

H	2.206033000	0.120669000	3.427735000
H	3.212535000	-1.029281000	2.513177000
H	2.234389000	-1.596464000	3.910281000
O	-1.307073000	-0.552413000	0.268523000
C	-1.754473000	-1.759188000	-0.039289000
C	-0.961250000	-2.646544000	-0.810151000
C	0.304589000	-2.157401000	-1.463215000
H	0.727202000	-2.981949000	-2.063885000
H	0.056972000	-1.353828000	-2.165776000
C	-3.016572000	-2.214935000	0.402646000
C	-3.421034000	-3.526697000	0.128228000
H	-4.396404000	-3.825027000	0.496239000
C	-2.633567000	-4.430219000	-0.589151000
C	-1.402868000	-3.944375000	-1.056832000
H	-0.760304000	-4.590327000	-1.650707000
C	-3.952234000	-1.252613000	1.164914000
O	2.616130000	0.885458000	0.432379000
C	3.752563000	0.278758000	0.130172000
C	3.782082000	-0.819179000	-0.755556000
C	2.528718000	-1.262890000	-1.460688000
H	2.175984000	-0.469178000	-2.131705000
H	2.772918000	-2.129652000	-2.099295000
C	4.977580000	0.717563000	0.693600000
C	6.158897000	0.051163000	0.378633000
H	7.075691000	0.420262000	0.829188000
C	6.208769000	-1.053700000	-0.487457000
C	4.993211000	-1.462362000	-1.038493000
H	4.957371000	-2.302866000	-1.724169000
C	-2.161539000	4.561548000	-0.024591000
H	-3.122039000	4.500462000	0.512458000
H	-1.640172000	5.426753000	0.412601000
Si	-2.622174000	4.981350000	-1.831643000
C	-1.198621000	5.789838000	-2.791721000
H	-0.845156000	6.692505000	-2.278609000
H	-0.348150000	5.110285000	-2.905525000
H	-1.532617000	6.086145000	-3.793642000
C	-4.055170000	6.233829000	-1.754242000
H	-3.761603000	7.140781000	-1.211903000
H	-4.368393000	6.536187000	-2.760794000
H	-4.928785000	5.808522000	-1.246021000
C	-3.214983000	3.417717000	-2.728345000
H	-2.422733000	2.661830000	-2.763596000
H	-4.078124000	2.976982000	-2.215167000
H	-3.516486000	3.644497000	-3.757867000

N	0.138527000	1.628398000	-1.752653000
C	0.621488000	2.842520000	-1.307035000
C	0.463754000	1.214290000	-2.996307000
C	1.665742000	3.480657000	-2.053433000
C	0.115672000	3.340310000	-0.083050000
C	1.359838000	1.863870000	-3.816777000
H	-0.029728000	0.303366000	-3.330687000
C	2.014048000	3.003650000	-3.291014000
H	2.128008000	4.375994000	-1.646702000
C	-1.355912000	3.275711000	0.286443000
H	1.570562000	1.493925000	-4.814625000
H	2.772170000	3.515990000	-3.879094000
H	-1.462017000	3.104618000	1.368234000
H	-1.838740000	2.420206000	-0.207658000
C	-5.244822000	-0.956067000	0.393986000
C	-5.204720000	-0.194737000	-0.773500000
C	-6.471748000	-1.440716000	0.829861000
C	-6.361872000	0.073521000	-1.482556000
H	-4.254515000	0.189021000	-1.124422000
C	-7.633985000	-1.172774000	0.120042000
H	-6.522963000	-2.031388000	1.735372000
C	-7.582632000	-0.415843000	-1.037243000
H	-8.487910000	-0.205319000	-1.591584000
C	-0.313693000	2.376172000	3.629793000
C	-1.005499000	2.508378000	4.848612000
C	-1.809098000	1.479957000	5.308936000
C	-1.921495000	0.324418000	4.534919000
C	-1.218401000	0.264075000	3.339757000
N	-0.429958000	1.250516000	2.877692000
H	-2.342987000	1.575298000	6.251032000
H	-0.889399000	3.425050000	5.419548000
H	-2.549953000	-0.507392000	4.836223000
H	-1.305686000	-0.602776000	2.696057000
C	0.511910000	3.476762000	3.160960000
H	0.276154000	4.451192000	3.584699000
C	1.482472000	3.373989000	2.234799000
H	2.039364000	4.254284000	1.927572000
H	1.895171000	2.436129000	1.879545000
H	0.586740000	4.273397000	0.216661000
C	7.578608000	-1.747833000	-0.790158000
C	-3.060553000	-5.904173000	-0.898039000
H	-8.581753000	-1.557303000	0.475154000
H	-6.314698000	0.667268000	-2.386765000
C	7.420660000	-2.947248000	-1.760533000

H	6.767492000	-3.706810000	-1.343569000
H	7.015729000	-2.628911000	-2.715483000
H	8.390351000	-3.400687000	-1.941261000
C	8.548973000	-0.722145000	-1.440477000
H	8.732492000	0.117406000	-0.778667000
H	9.502154000	-1.193106000	-1.662148000
H	8.133320000	-0.340071000	-2.367881000
C	8.200221000	-2.274459000	0.534029000
H	9.150011000	-2.762701000	0.336738000
H	8.376040000	-1.464587000	1.233847000
H	7.538993000	-2.994924000	1.005956000
C	-3.148160000	-6.110855000	-2.436296000
H	-2.189751000	-5.930794000	-2.911343000
H	-3.452256000	-7.128424000	-2.663444000
H	-3.876138000	-5.432242000	-2.870268000
C	-2.009360000	-6.885753000	-0.307308000
H	-2.297527000	-7.913296000	-0.508589000
H	-1.029441000	-6.719527000	-0.741821000
H	-1.931258000	-6.759004000	0.768280000
C	-4.442016000	-6.248929000	-0.283546000
H	-4.430345000	-6.137123000	0.795688000
H	-5.221449000	-5.612219000	-0.688766000
H	-4.696511000	-7.279217000	-0.512408000
C	4.970038000	1.931299000	1.628311000
H	4.510726000	2.788177000	1.141332000
H	4.402704000	1.727617000	2.534346000
H	5.981292000	2.200962000	1.916288000
H	-3.416654000	-0.321004000	1.331009000
H	-4.207496000	-1.670739000	2.137604000

TS2^P_{syn}, $E_{\text{(SCF Done)}} = -2465.421545 \text{ a.u.}$ IF = $i202.11 \text{ cm}^{-1}$

Y	0.264299000	-0.222077000	0.287307000
N	-0.340218000	2.351107000	0.016703000
C	-0.012323000	2.797838000	-1.349921000
H	1.045416000	3.077465000	-1.367446000
H	-0.591985000	3.694301000	-1.625928000
C	-0.261558000	1.705292000	-2.377771000
H	-1.306821000	1.394608000	-2.386907000
H	0.004224000	2.061692000	-3.381505000
O	0.503132000	0.530253000	-2.075460000
C	1.793784000	0.498232000	-2.686109000
H	2.224443000	-0.474731000	-2.449367000
H	2.441158000	1.292640000	-2.298545000
H	1.687142000	0.594075000	-3.773569000

O	-1.842193000	-0.171007000	-0.105157000
C	-2.863587000	0.547665000	-0.544658000
C	-2.836516000	1.954908000	-0.456081000
C	-1.761085000	2.631811000	0.348762000
H	-1.918266000	3.723302000	0.298990000
H	-1.876996000	2.360164000	1.407105000
C	-4.005937000	-0.064189000	-1.116963000
C	-5.019059000	0.736941000	-1.640821000
H	-5.871660000	0.233106000	-2.086469000
C	-4.982675000	2.140721000	-1.618397000
C	-3.874177000	2.720293000	-0.997650000
H	-3.797265000	3.799061000	-0.905367000
C	-4.134965000	-1.598055000	-1.096658000
O	2.124078000	0.820341000	0.610775000
C	2.705690000	2.014961000	0.622649000
C	1.934967000	3.182210000	0.796570000
C	0.462406000	3.072031000	1.053162000
H	0.279646000	2.541014000	1.999834000
H	0.051273000	4.087014000	1.181387000
C	4.105831000	2.167145000	0.455219000
C	4.662659000	3.444245000	0.458412000
H	5.738485000	3.515263000	0.329448000
C	3.909501000	4.617746000	0.622906000
C	2.535838000	4.446399000	0.788716000
H	1.886689000	5.304776000	0.927638000
C	4.747146000	-3.393748000	-0.671742000
H	5.598067000	-2.763467000	-0.975315000
H	5.129182000	-4.013266000	0.154149000
Si	4.386021000	-4.547342000	-2.151953000
C	3.457622000	-6.123259000	-1.644371000
H	3.982259000	-6.644370000	-0.834506000
H	2.440903000	-5.901360000	-1.304114000
H	3.385421000	-6.815283000	-2.492467000
C	6.067349000	-5.063473000	-2.880288000
H	6.682502000	-5.578967000	-2.133001000
H	5.935819000	-5.745255000	-3.729013000
H	6.633026000	-4.193625000	-3.234880000
C	3.398232000	-3.622053000	-3.484770000
H	2.423196000	-3.304891000	-3.098867000
H	3.937710000	-2.731595000	-3.830598000
H	3.222425000	-4.263945000	-4.356129000
N	0.683691000	-2.318056000	-0.847598000
C	1.223171000	-3.344552000	-0.073741000
C	-0.342415000	-2.620817000	-1.683937000

C	0.449207000	-4.541842000	0.083192000
C	2.490979000	-3.216754000	0.518526000
C	-0.983243000	-3.838313000	-1.720945000
H	-0.669006000	-1.802385000	-2.321533000
C	-0.611763000	-4.796321000	-0.746380000
H	0.785731000	-5.281232000	0.805138000
C	3.624874000	-2.475079000	-0.142103000
H	-1.783084000	-4.023717000	-2.429177000
H	-1.151290000	-5.737619000	-0.670456000
H	4.085502000	-1.762046000	0.555032000
H	3.224982000	-1.864808000	-0.960655000
C	-4.490630000	-2.132320000	0.299962000
C	-3.629186000	-2.986562000	0.979426000
C	-5.692211000	-1.775082000	0.910299000
C	-3.956860000	-3.470224000	2.238900000
H	-2.699070000	-3.287632000	0.514844000
C	-6.021047000	-2.257276000	2.164777000
H	-6.375259000	-1.112336000	0.394934000
C	-5.152371000	-3.107157000	2.834936000
H	-5.410201000	-3.485620000	3.815462000
C	0.157857000	-1.661759000	3.573576000
C	-0.566872000	-1.958927000	4.759891000
C	-1.770472000	-1.353714000	5.033255000
C	-2.294302000	-0.444886000	4.100668000
C	-1.572888000	-0.228911000	2.943723000
N	-0.379131000	-0.795334000	2.650925000
H	-2.305871000	-1.580440000	5.951978000
H	-0.130199000	-2.665266000	5.459980000
H	-3.248131000	0.050219000	4.248705000
H	-1.991923000	0.401618000	2.167944000
C	1.436228000	-2.274542000	3.403843000
H	1.655947000	-3.066166000	4.117749000
C	2.387111000	-1.980290000	2.457725000
H	2.794571000	-4.102772000	1.075379000
C	4.994596000	0.932688000	0.290307000
H	4.684486000	0.338261000	-0.565187000
H	3.383858000	-2.387467000	2.594208000
H	2.377625000	-1.041653000	1.906959000
C	4.620381000	6.011802000	0.620040000
C	-6.155646000	2.963280000	-2.248763000
H	-6.959330000	-1.971403000	2.623164000
H	-3.275121000	-4.137555000	2.751019000
H	6.029830000	1.225080000	0.146564000
H	4.938961000	0.296801000	1.170248000

H	-4.909177000	-1.897640000	-1.801830000
H	-3.200387000	-2.051696000	-1.415582000
C	3.614550000	7.176148000	0.813951000
H	2.878779000	7.196930000	0.016681000
H	3.094858000	7.092038000	1.762720000
H	4.146134000	8.122625000	0.804959000
C	5.350886000	6.221414000	-0.736098000
H	5.845149000	7.188250000	-0.751867000
H	6.101588000	5.455696000	-0.899392000
H	4.644129000	6.186982000	-1.559682000
C	5.657254000	6.067701000	1.776856000
H	6.414987000	5.300260000	1.661171000
H	6.153231000	7.033715000	1.791309000
H	5.167494000	5.921245000	2.734744000
C	-5.925293000	4.491843000	-2.124054000
H	-5.863165000	4.796462000	-1.084515000
H	-5.013501000	4.794194000	-2.628693000
H	-6.754096000	5.023948000	-2.580586000
C	-6.282361000	2.613132000	-3.758129000
H	-6.490105000	1.557964000	-3.899548000
H	-7.090766000	3.180513000	-4.209674000
H	-5.363064000	2.852774000	-4.283882000
C	-7.486442000	2.612210000	-1.526061000
H	-7.721693000	1.558299000	-1.628154000
H	-7.418509000	2.845370000	-0.467796000
H	-8.306777000	3.184239000	-1.949373000

TS2^q_{iso}, $E_{\text{(SCF Done)}} = -2603.795468$ a.u. **IF** = *i*54.89 cm⁻¹

Y	-0.111765000	-0.481462000	0.380570000
N	-1.568315000	1.505450000	-0.610047000
C	-2.162302000	2.339898000	0.453320000
H	-3.145980000	1.926663000	0.695400000
H	-2.318334000	3.373399000	0.104799000
C	-1.304056000	2.355948000	1.707120000
H	-0.320166000	2.784985000	1.513606000
H	-1.790347000	2.945980000	2.495760000
O	-1.074009000	1.024639000	2.180232000
C	-2.080536000	0.536832000	3.065407000
H	-1.764902000	-0.456903000	3.384591000
H	-3.054024000	0.462793000	2.568946000
H	-2.151913000	1.195464000	3.940242000
O	1.303340000	1.112663000	0.093360000
C	1.465709000	2.379194000	-0.248320000
C	0.442387000	3.067845000	-0.952830000

C	-0.735379000	2.326077000	-1.526768000
H	-1.392211000	3.057607000	-2.028654000
H	-0.390729000	1.642294000	-2.312203000
C	2.641414000	3.088170000	0.082004000
C	2.733616000	4.454786000	-0.226500000
H	3.645360000	4.967734000	0.048293000
C	1.714426000	5.165706000	-0.865586000
C	0.579330000	4.425681000	-1.227887000
H	-0.232257000	4.914499000	-1.762903000
O	-2.114120000	-1.249857000	0.328882000
C	-3.383065000	-0.927297000	0.121928000
C	-3.714373000	0.148010000	-0.725586000
C	-2.625829000	0.874706000	-1.461819000
H	-2.100228000	0.186794000	-2.139456000
H	-3.086095000	1.652686000	-2.094010000
C	-4.435831000	-1.638456000	0.749539000
C	-5.753674000	-1.249216000	0.519622000
H	-6.533984000	-1.817386000	1.017282000
C	-6.106741000	-0.176763000	-0.316263000
C	-5.052677000	0.504959000	-0.926261000
H	-5.249017000	1.340550000	-1.590233000
C	3.399302000	-4.562876000	-0.176776000
H	4.248869000	-4.360722000	0.494103000
H	3.050412000	-5.572117000	0.091323000
Si	4.110078000	-4.626356000	-1.949057000
C	2.940784000	-5.492427000	-3.169540000
H	2.668502000	-6.493596000	-2.814167000
H	2.018334000	-4.919478000	-3.310097000
H	3.421939000	-5.606094000	-4.148770000
C	5.731526000	-5.621853000	-1.872229000
H	5.553065000	-6.640337000	-1.506757000
H	6.193799000	-5.700286000	-2.863487000
H	6.458527000	-5.149043000	-1.201193000
C	4.485419000	-2.870006000	-2.564664000
H	3.571305000	-2.267428000	-2.608440000
H	5.193807000	-2.360052000	-1.900817000
H	4.924147000	-2.892482000	-3.569315000
N	0.662576000	-1.646948000	-1.554620000
C	0.405947000	-3.018904000	-1.543197000
C	0.445680000	-0.966933000	-2.711183000
C	-0.449979000	-3.543930000	-2.577719000
C	0.993485000	-3.841313000	-0.582791000
C	-0.208103000	-1.480685000	-3.805606000
H	0.822427000	0.054894000	-2.713836000

C	-0.733579000	-2.797393000	-3.687276000
H	-0.796586000	-4.570687000	-2.490894000
C	2.281290000	-3.539036000	0.120974000
H	-0.340580000	-0.889437000	-4.705446000
H	-1.334244000	-3.219093000	-4.489987000
H	2.135152000	-3.528479000	1.215208000
H	2.617926000	-2.531063000	-0.153608000
C	0.753875000	-2.637781000	3.139388000
C	1.367147000	-2.797470000	4.407585000
C	1.990127000	-1.742593000	5.035659000
C	2.023955000	-0.499472000	4.388323000
C	1.409955000	-0.397748000	3.154911000
N	0.772419000	-1.412048000	2.526032000
H	2.452362000	-1.875621000	6.010504000
H	1.331246000	-3.777372000	4.874560000
H	2.519082000	0.361042000	4.824537000
H	1.431702000	0.546391000	2.618642000
C	0.160460000	-3.800928000	2.530244000
H	0.443092000	-4.738254000	3.006488000
C	-0.622245000	-3.854992000	1.419772000
H	-0.995569000	-4.817216000	1.082716000
H	-1.131894000	-2.999680000	0.993710000
H	0.740460000	-4.897220000	-0.669924000
C	-4.108149000	-2.830142000	1.654307000
H	-3.670149000	-3.643293000	1.080137000
H	-3.393380000	-2.552724000	2.425806000
C	-7.614557000	0.189683000	-0.521697000
C	1.793073000	6.692349000	-1.201403000
H	-5.005943000	-3.201601000	2.138187000
C	4.122441000	2.526153000	2.895057000
H	4.290434000	3.572161000	3.109437000
H	3.166627000	2.251698000	3.316085000
H	4.890231000	1.954062000	3.396995000
C	5.825025000	3.041029000	0.266439000
H	5.870547000	4.090617000	0.518945000
H	6.692654000	2.557181000	0.692579000
H	5.884396000	2.949999000	-0.808797000
Si	4.170584000	2.206713000	0.947762000
C	4.289924000	0.277471000	0.587141000
H	3.620031000	-0.279325000	1.225746000
H	4.027142000	0.071635000	-0.440711000
H	5.296718000	-0.077606000	0.760499000
C	-7.793190000	1.400061000	-1.474634000
H	-7.305936000	2.285981000	-1.080726000

H	-7.385738000	1.188952000	-2.457832000
H	-8.849840000	1.621074000	-1.589231000
C	-8.365596000	-1.025647000	-1.134288000
H	-8.312797000	-1.889207000	-0.480090000
H	-9.412471000	-0.781912000	-1.289365000
H	-7.932782000	-1.297086000	-2.092314000
C	-8.254103000	0.552035000	0.848260000
H	-9.300222000	0.812881000	0.718221000
H	-8.197654000	-0.281424000	1.540162000
H	-7.744950000	1.400806000	1.294788000
C	1.702155000	6.893599000	-2.740259000
H	0.765749000	6.510590000	-3.131547000
H	1.764563000	7.949498000	-2.986425000
H	2.516445000	6.378049000	-3.240214000
C	0.613032000	7.436744000	-0.515299000
H	0.659195000	8.499322000	-0.734628000
H	-0.343381000	7.062187000	-0.864140000
H	0.656732000	7.309549000	0.562175000
C	3.118175000	7.328394000	-0.707033000
H	3.224269000	7.228945000	0.368261000
H	3.976765000	6.867249000	-1.183798000
H	3.127229000	8.386496000	-0.949699000

TS2^o_{syn}, $E_{(\text{SCF Done})} = -2603.789384 \text{ a.u.}$ IF = $i203.36 \text{ cm}^{-1}$

Y	0.297429000	-0.288985000	0.434670000
N	-0.735109000	2.120055000	0.223248000
C	-0.848830000	2.485879000	-1.204947000
H	0.079184000	2.987593000	-1.494921000
H	-1.669481000	3.203248000	-1.364807000
C	-1.073189000	1.284365000	-2.117262000
H	-2.008438000	0.771981000	-1.898763000
H	-1.103753000	1.620133000	-3.162173000
O	-0.033208000	0.301924000	-1.974772000
C	1.064412000	0.518571000	-2.862872000
H	1.793666000	-0.269122000	-2.677343000
H	1.536147000	1.490716000	-2.685740000
H	0.710871000	0.451112000	-3.899095000
O	-1.852953000	-0.584377000	0.371689000
C	-3.008071000	0.008357000	0.099838000
C	-3.167550000	1.397442000	0.333719000
C	-2.045547000	2.207497000	0.917214000
H	-2.358533000	3.265501000	0.941754000
H	-1.858776000	1.926729000	1.961535000
C	-4.089750000	-0.696336000	-0.476312000

C	-5.290339000	-0.019500000	-0.741968000
H	-6.099944000	-0.591205000	-1.173173000
C	-5.477477000	1.341986000	-0.487357000
C	-4.374635000	2.026061000	0.041297000
H	-4.446646000	3.093468000	0.238926000
O	1.975440000	1.023909000	0.089792000
C	2.355472000	2.286384000	-0.069353000
C	1.498052000	3.338303000	0.310302000
C	0.187209000	3.030384000	0.971550000
H	0.356782000	2.552737000	1.948174000
H	-0.333694000	3.980642000	1.174307000
C	3.616790000	2.624336000	-0.623381000
C	3.955239000	3.966869000	-0.782592000
H	4.931132000	4.184175000	-1.206173000
C	3.110106000	5.027937000	-0.420889000
C	1.877213000	4.672561000	0.125655000
H	1.171569000	5.436420000	0.435585000
C	3.992167000	-2.803347000	-1.957526000
H	4.079328000	-2.178389000	-2.860776000
H	5.012982000	-2.870060000	-1.552268000
Si	3.464104000	-4.543470000	-2.549394000
C	3.791895000	-5.889083000	-1.251875000
H	4.839775000	-5.882452000	-0.928980000
H	3.162644000	-5.744121000	-0.367783000
H	3.576138000	-6.882354000	-1.664106000
C	4.487269000	-4.940778000	-4.104226000
H	5.562033000	-4.922426000	-3.887140000
H	4.243783000	-5.936927000	-4.492421000
H	4.295870000	-4.215059000	-4.903715000
C	1.619801000	-4.535100000	-3.002116000
H	1.001355000	-4.324782000	-2.122397000
H	1.398201000	-3.776154000	-3.762504000
H	1.311796000	-5.507814000	-3.403567000
N	0.661858000	-2.693273000	0.721337000
C	1.896947000	-3.248953000	1.014001000
C	-0.438094000	-3.223814000	1.306612000
C	1.968539000	-4.262031000	2.020669000
C	3.065935000	-2.752918000	0.419995000
C	-0.424637000	-4.255048000	2.221343000
H	-1.372267000	-2.745645000	1.033131000
C	0.833344000	-4.763091000	2.605210000
H	2.948799000	-4.647155000	2.287513000
C	3.087739000	-2.090374000	-0.930092000
H	-1.350233000	-4.623642000	2.649837000

H	0.905275000	-5.549874000	3.353191000
H	3.408934000	-1.041688000	-0.861129000
H	2.057224000	-2.066083000	-1.325893000
C	1.578981000	-0.806355000	3.724650000
C	1.346058000	-0.900356000	5.127345000
C	0.134212000	-0.569391000	5.684053000
C	-0.908894000	-0.151476000	4.841261000
C	-0.639762000	-0.094246000	3.488717000
N	0.550606000	-0.378163000	2.914883000
H	-0.014740000	-0.642963000	6.758643000
H	2.165002000	-1.238302000	5.755567000
H	-1.898012000	0.088649000	5.215976000
H	-1.443289000	0.151714000	2.799256000
C	2.878946000	-1.172664000	3.251283000
H	3.493882000	-1.651425000	4.011071000
C	3.421802000	-1.030052000	1.994141000
H	3.975987000	-3.286359000	0.688986000
C	4.601951000	1.524321000	-1.031313000
H	4.212532000	0.931085000	-1.855430000
H	4.481980000	-1.231674000	1.872793000
H	3.014902000	-0.332273000	1.270797000
C	3.575433000	6.506804000	-0.634156000
C	-6.811536000	2.108735000	-0.773380000
H	5.545215000	1.959071000	-1.346049000
H	4.796849000	0.848871000	-0.202824000
C	-2.280264000	-2.954964000	-1.979738000
H	-2.141913000	-2.202749000	-2.743811000
H	-1.408471000	-2.959928000	-1.342893000
H	-2.347521000	-3.918707000	-2.465419000
C	-5.440276000	-3.081598000	-2.108430000
H	-6.378836000	-2.988782000	-1.581044000
H	-5.481087000	-2.451155000	-2.985211000
H	-5.344689000	-4.106563000	-2.438337000
C	-4.020068000	-3.745006000	0.650637000
H	-5.053496000	-3.922752000	0.913044000
H	-3.548883000	-4.701024000	0.470013000
H	-3.536027000	-3.282631000	1.498040000
Si	-3.917659000	-2.596103000	-0.949580000
C	4.871080000	6.766465000	0.184539000
H	5.673504000	6.109367000	-0.133023000
H	5.201007000	7.792504000	0.051270000
H	4.692931000	6.600004000	1.242559000
C	3.862605000	6.749972000	-2.142540000
H	4.182209000	7.775150000	-2.304268000

H	4.645127000	6.091421000	-2.503816000
H	2.969283000	6.574618000	-2.734335000
C	2.499624000	7.525172000	-0.175342000
H	1.577717000	7.401663000	-0.734158000
H	2.281164000	7.415953000	0.881849000
H	2.859887000	8.535701000	-0.341182000
C	-6.550716000	3.242934000	-1.804304000
H	-5.825753000	3.956739000	-1.427899000
H	-6.173298000	2.832178000	-2.735887000
H	-7.471594000	3.777886000	-2.016641000
C	-7.346866000	2.728516000	0.548037000
H	-8.277476000	3.257707000	0.365698000
H	-7.534437000	1.952518000	1.283903000
H	-6.635672000	3.431539000	0.968317000
C	-7.907142000	1.173976000	-1.348305000
H	-7.596405000	0.737831000	-2.291947000
H	-8.140743000	0.371651000	-0.656226000
H	-8.815280000	1.742336000	-1.523682000

TS2^R_{iso}, $E_{\text{(SCF Done)}} = -2426.132166$ a.u. IF = $i86.97$ cm⁻¹

Y	-0.100265000	-0.475144000	0.323007000
N	-1.701824000	1.406828000	-0.688182000
C	-2.271386000	2.270720000	0.365165000
H	-3.216157000	1.824598000	0.689702000
H	-2.502577000	3.274294000	-0.026805000
C	-1.343166000	2.401577000	1.561668000
H	-0.401657000	2.879903000	1.287385000
H	-1.819005000	3.003102000	2.347943000
O	-0.999908000	1.115340000	2.086424000
C	-1.902620000	0.623517000	3.075093000
H	-1.489953000	-0.318923000	3.437250000
H	-2.899602000	0.444441000	2.658317000
H	-1.962363000	1.336969000	3.906621000
O	1.216084000	1.104078000	-0.270489000
C	1.288002000	2.393235000	-0.556348000
C	0.202675000	3.033486000	-1.201966000
C	-0.957392000	2.211785000	-1.694829000
H	-1.672072000	2.881399000	-2.203998000
H	-0.607414000	1.501444000	-2.454329000
C	2.407945000	3.178281000	-0.186550000
C	2.395717000	4.558639000	-0.448851000
H	3.274907000	5.119233000	-0.154242000
C	1.331226000	5.207639000	-1.076981000
C	0.240492000	4.403544000	-1.444451000

H	-0.612902000	4.851005000	-1.948749000
O	-2.070839000	-1.299705000	0.472597000
C	-3.360990000	-1.051674000	0.299877000
C	-3.786504000	-0.049541000	-0.595137000
C	-2.779177000	0.684806000	-1.435047000
H	-2.267794000	-0.017055000	-2.108894000
H	-3.313427000	1.406008000	-2.076584000
C	-4.344921000	-1.778629000	1.014654000
C	-5.691022000	-1.476104000	0.823863000
H	-6.416386000	-2.054968000	1.387911000
C	-6.138196000	-0.476201000	-0.055990000
C	-5.150707000	0.222210000	-0.752465000
H	-5.422330000	1.003522000	-1.454969000
C	3.681662000	-4.221582000	-0.198412000
H	4.563811000	-3.875184000	0.362627000
H	3.490882000	-5.243957000	0.162593000
Si	4.212004000	-4.322918000	-2.030881000
C	3.056303000	-5.424314000	-3.059461000
H	2.966442000	-6.423130000	-2.615495000
H	2.052220000	-4.993535000	-3.130824000
H	3.446054000	-5.546236000	-4.077523000
C	5.954631000	-5.089353000	-2.075916000
H	5.958885000	-6.094055000	-1.636066000
H	6.319913000	-5.177090000	-3.106141000
H	6.673785000	-4.478034000	-1.517859000
C	4.276520000	-2.582320000	-2.785696000
H	3.287080000	-2.111935000	-2.766430000
H	4.967205000	-1.934532000	-2.232506000
H	4.614139000	-2.617684000	-3.828411000
N	0.499877000	-1.843189000	-1.555355000
C	0.408524000	-3.214736000	-1.338971000
C	0.052230000	-1.348420000	-2.736413000
C	-0.466408000	-3.970091000	-2.195909000
C	1.166136000	-3.829278000	-0.335084000
C	-0.650774000	-2.071857000	-3.671032000
H	0.280025000	-0.296720000	-2.905262000
C	-0.970100000	-3.415362000	-3.340723000
H	-0.656309000	-5.011850000	-1.950306000
C	2.482615000	-3.317579000	0.167773000
H	-0.970818000	-1.618516000	-4.603056000
H	-1.589245000	-4.009670000	-4.008723000
H	2.462590000	-3.235451000	1.267935000
H	2.657389000	-2.301769000	-0.211696000
C	1.194115000	-2.214523000	3.172526000

C	1. 946663000	-2. 188486000	4. 374837000
C	2. 582140000	-1. 041164000	4. 792372000
C	2. 485311000	0. 111766000	3. 998471000
C	1. 730642000	0. 036155000	2. 844297000
N	1. 078114000	-1. 072039000	2. 421922000
H	3. 155472000	-1. 034362000	5. 716000000
H	2. 012343000	-3. 102327000	4. 958152000
H	2. 987200000	1. 037190000	4. 260262000
H	1. 648935000	0. 905022000	2. 198204000
C	0. 610329000	-3. 462188000	2. 762512000
H	0. 976666000	-4. 325703000	3. 314953000
C	-0. 241551000	-3. 680492000	1. 718742000
H	-0. 602445000	-4. 687790000	1. 534957000
H	-0. 853399000	-2. 909198000	1. 266032000
H	1. 038885000	-4. 909767000	-0. 276056000
C	-7. 671445000	-0. 204148000	-0. 214568000
C	-3. 905303000	-2. 894482000	1. 967372000
H	-3. 405246000	-3. 692089000	1. 422776000
H	-3. 207393000	-2. 521411000	2. 713856000
H	-4. 761509000	-3. 318416000	2. 482485000
C	1. 310250000	6. 741334000	-1. 390501000
C	3. 596492000	2. 545754000	0. 497063000
C	4. 145660000	1. 349778000	0. 027744000
C	4. 187449000	3. 152224000	1. 606152000
C	5. 243089000	0. 779839000	0. 652828000
H	3. 715830000	0. 871238000	-0. 842508000
C	5. 286048000	2. 583002000	2. 229246000
H	3. 778991000	4. 078483000	1. 988222000
C	5. 816920000	1. 393807000	1. 756113000
H	5. 656664000	-0. 145217000	0. 271448000
H	5. 728626000	3. 069821000	3. 089011000
H	6. 675137000	0. 948453000	2. 242352000
C	-8. 377697000	-1. 492871000	-0. 721341000
H	-8. 249485000	-2. 311167000	-0. 021025000
H	-9. 442123000	-1. 315476000	-0. 843542000
H	-7. 970257000	-1. 798225000	-1. 680288000
C	-8. 272905000	0. 205466000	1. 159286000
H	-9. 336581000	0. 401234000	1. 061351000
H	-8. 140746000	-0. 580363000	1. 895199000
H	-7. 794291000	1. 105868000	1. 532423000
C	-7. 957481000	0. 935014000	-1. 227262000
H	-7. 504546000	1. 867955000	-0. 908042000
H	-7. 580547000	0. 686827000	-2. 213970000
H	-9. 028740000	1. 091861000	-1. 306595000

C	0.091728000	7.400891000	-0.685205000
H	-0.842449000	6.972661000	-1.032467000
H	0.151958000	7.262027000	0.390038000
H	0.070172000	8.467177000	-0.889701000
C	1.193778000	6.956189000	-2.925731000
H	1.186775000	8.017034000	-3.157964000
H	2.035071000	6.500183000	-3.438667000
H	0.280407000	6.519188000	-3.314892000
C	2.597183000	7.452429000	-0.897697000
H	2.716446000	7.349391000	0.175866000
H	3.479146000	7.049294000	-1.384285000
H	2.539754000	8.511397000	-1.129608000

TS2^R_{syn}, $E_{(\text{SCF Done})} = -2426.129674 \text{ a.u.}$ IF = *i*164.48 cm⁻¹

Y	0.215911000	-0.204161000	0.500790000
N	-0.335083000	2.369485000	0.138033000
C	-0.204227000	2.722391000	-1.287801000
H	0.845739000	2.962282000	-1.480489000
H	-0.794202000	3.621093000	-1.532424000
C	-0.634844000	1.579882000	-2.194258000
H	-1.684016000	1.323824000	-2.044648000
H	-0.491732000	1.856523000	-3.246820000
O	0.113689000	0.390252000	-1.911188000
C	1.293908000	0.237146000	-2.701175000
H	1.712624000	-0.736170000	-2.445019000
H	2.024911000	1.023998000	-2.484490000
H	1.027299000	0.250786000	-3.765014000
O	-1.937624000	-0.083592000	0.471658000
C	-2.973171000	0.636405000	0.073269000
C	-2.874828000	2.046036000	0.036505000
C	-1.682615000	2.717601000	0.658617000
H	-1.814096000	3.810759000	0.579856000
H	-1.653419000	2.493699000	1.733623000
C	-4.193958000	0.044478000	-0.349007000
C	-5.202850000	0.867671000	-0.866464000
H	-6.121305000	0.382808000	-1.182147000
C	-5.095433000	2.261037000	-0.967086000
C	-3.910971000	2.824260000	-0.483455000
H	-3.771492000	3.900839000	-0.488204000
O	2.134194000	0.782590000	0.470990000
C	2.749196000	1.948656000	0.304768000
C	2.052313000	3.155446000	0.514125000
C	0.634519000	3.117165000	0.997161000
H	0.583151000	2.645944000	1.990473000

H	0.277358000	4.152556000	1.123405000
C	4.107819000	2.030634000	-0.093627000
C	4.696174000	3.281341000	-0.269019000
H	5.738385000	3.299174000	-0.573230000
C	4.015760000	4.493353000	-0.070210000
C	2.681745000	4.390628000	0.322320000
H	2.089117000	5.282309000	0.499143000
C	4.408045000	-3.632412000	-0.751812000
H	5.237018000	-3.078644000	-1.220552000
H	4.862123000	-4.166632000	0.096834000
Si	3.839993000	-4.929155000	-2.036140000
C	2.857143000	-6.352060000	-1.256400000
H	3.422847000	-6.820395000	-0.442072000
H	1.904321000	-5.998505000	-0.849526000
H	2.641290000	-7.127333000	-2.001701000
C	5.408316000	-5.653185000	-2.836092000
H	6.057112000	-6.119662000	-2.085034000
H	5.154716000	-6.420151000	-3.577677000
H	5.992244000	-4.877067000	-3.345018000
C	2.793442000	-4.086141000	-3.379254000
H	1.874773000	-3.669960000	-2.951051000
H	3.349718000	-3.270785000	-3.857842000
H	2.506811000	-4.799312000	-4.161101000
N	0.376972000	-2.352282000	-0.543812000
C	0.965223000	-3.324703000	0.266101000
C	-0.779820000	-2.669074000	-1.187368000
C	0.152255000	-4.435228000	0.675765000
C	2.311091000	-3.229096000	0.647375000
C	-1.484237000	-3.831778000	-0.988176000
H	-1.150771000	-1.904029000	-1.865860000
C	-1.031439000	-4.697836000	0.038107000
H	0.546467000	-5.112251000	1.429085000
C	3.374012000	-2.614151000	-0.223332000
H	-2.395139000	-4.028300000	-1.541798000
H	-1.610784000	-5.579218000	0.303844000
H	3.927315000	-1.832011000	0.314591000
H	2.894440000	-2.101885000	-1.066494000
C	0.570501000	-1.313297000	3.927880000
C	0.035577000	-1.476481000	5.233477000
C	-1.122345000	-0.840398000	5.615685000
C	-1.787387000	-0.038774000	4.676750000
C	-1.243538000	0.053397000	3.410484000
N	-0.098979000	-0.544892000	3.008082000
H	-1.514013000	-0.963382000	6.622377000

H	0.578388000	-2.106566000	5.932065000
H	-2.713932000	0.475082000	4.909706000
H	-1.774230000	0.600760000	2.640720000
C	1.806659000	-1.969418000	3.629468000
H	2.116903000	-2.705303000	4.368830000
C	2.600169000	-1.786506000	2.531422000
H	2.647279000	-4.058731000	1.267872000
H	3.579520000	-2.252778000	2.516363000
H	2.519322000	-0.912656000	1.889491000
C	4.759432000	5.853095000	-0.286522000
C	-6.276529000	3.097099000	-1.563895000
C	-4.445847000	-1.437015000	-0.201074000
C	-4.138382000	-2.097101000	0.990440000
C	-5.056919000	-2.167254000	-1.220949000
C	-4.435419000	-3.440116000	1.155687000
H	-3.681159000	-1.546204000	1.801548000
C	-5.353164000	-3.510319000	-1.055902000
H	-5.302390000	-1.678025000	-2.154287000
C	-5.045671000	-4.151316000	0.133849000
H	-4.196322000	-3.931903000	2.090091000
H	-5.827536000	-4.058891000	-1.859756000
H	-5.280244000	-5.199778000	0.264261000
C	4.919662000	0.752485000	-0.313712000
H	5.003357000	0.183939000	0.609117000
H	4.447261000	0.111228000	-1.053251000
H	5.920912000	0.991724000	-0.657449000
C	5.971752000	5.941390000	0.682457000
H	6.676417000	5.136662000	0.502545000
H	6.493248000	6.884410000	0.547781000
H	5.639941000	5.879329000	1.714401000
C	3.834826000	7.068877000	-0.018378000
H	2.980814000	7.068393000	-0.687772000
H	3.473049000	7.068840000	1.004577000
H	4.387010000	7.989563000	-0.179357000
C	5.266101000	5.942080000	-1.753546000
H	5.780566000	6.884277000	-1.917586000
H	5.956569000	5.136583000	-1.979311000
H	4.434286000	5.882881000	-2.448927000
C	-5.950019000	4.612633000	-1.606982000
H	-5.776609000	5.006167000	-0.610835000
H	-5.072267000	4.808185000	-2.214320000
H	-6.785600000	5.153509000	-2.040234000
C	-7.548711000	2.898047000	-0.693049000
H	-7.848522000	1.855838000	-0.670299000

H	-7.366935000	3.222682000	0.326975000
H	-8.373969000	3.479068000	-1.093997000
C	-6.567583000	2.622620000	-3.015420000
H	-5.691035000	2.753374000	-3.642749000
H	-6.848222000	1.575115000	-3.036651000
H	-7.381937000	3.199406000	-3.443705000

TS2^s_{iso}, $E_{\text{(SCF Done)}} = -3313.413141 \text{ a.u.}$ IF = $i69.16 \text{ cm}^{-1}$

Y	1.358291000	-0.395698000	0.231257000
N	1.450942000	-2.609687000	-1.185210000
C	1.226047000	-3.806563000	-0.351365000
H	2.199370000	-4.156422000	0.004234000
H	0.783093000	-4.623806000	-0.943519000
C	0.328397000	-3.513172000	0.838426000
H	-0.658982000	-3.193954000	0.512147000
H	0.216358000	-4.412168000	1.459286000
O	0.847850000	-2.444188000	1.638246000
C	1.773711000	-2.865699000	2.639061000
H	2.051237000	-1.976813000	3.206468000
H	2.673676000	-3.305865000	2.197393000
H	1.289328000	-3.588969000	3.307168000
O	-0.682728000	-0.675916000	-0.419775000
C	-1.528594000	-1.446060000	-1.093020000
C	-1.010905000	-2.453067000	-1.943494000
C	0.457052000	-2.508706000	-2.281981000
H	0.613384000	-3.361166000	-2.965491000
H	0.733812000	-1.612205000	-2.850323000
C	-2.952858000	-1.302131000	-0.999721000
C	-3.750318000	-2.200661000	-1.706654000
H	-4.828602000	-2.123800000	-1.677499000
C	-3.227769000	-3.231704000	-2.498930000
C	-1.847926000	-3.347251000	-2.619643000
H	-1.398707000	-4.102070000	-3.254132000
C	-3.604355000	-0.141391000	-0.140583000
O	3.360541000	-1.153010000	0.457891000
C	4.191866000	-2.147568000	0.174403000
C	3.951171000	-2.963952000	-0.954819000
C	2.787843000	-2.660947000	-1.853377000
H	2.926447000	-1.687639000	-2.343829000
H	2.756610000	-3.417453000	-2.655537000
C	5.315692000	-2.431795000	0.985050000
C	6.165178000	-3.496138000	0.659922000
H	7.016561000	-3.682945000	1.301747000
C	5.925653000	-4.295215000	-0.461167000

C	4. 806096000	-4. 019629000	-1. 257842000
H	4. 622063000	-4. 648926000	-2. 125334000
C	2. 666717000	5. 137541000	0. 599677000
H	1. 872031000	5. 668075000	1. 146074000
H	3. 546399000	5. 176990000	1. 261019000
Si	3. 056375000	6. 198540000	-0. 941483000
C	4. 690588000	5. 713013000	-1. 782643000
H	5. 521306000	5. 699613000	-1. 066854000
H	4. 621338000	4. 721291000	-2. 241762000
H	4. 942069000	6. 433779000	-2. 570430000
C	3. 206481000	8. 002745000	-0. 351604000
H	4. 000433000	8. 110243000	0. 397324000
H	3. 444033000	8. 673160000	-1. 186170000
H	2. 271299000	8. 352274000	0. 101893000
C	1. 653519000	6. 079293000	-2. 214925000
H	1. 517675000	5. 045420000	-2. 551805000
H	0. 701900000	6. 429010000	-1. 797929000
H	1. 875879000	6. 692115000	-3. 096651000
N	1. 896115000	1. 297069000	-1. 383087000
C	3. 138427000	1. 919901000	-1. 221559000
C	1. 573104000	0. 848326000	-2. 626848000
C	4. 157590000	1. 628655000	-2. 197336000
C	3. 342581000	2. 829680000	-0. 186590000
C	2. 460224000	0. 755616000	-3. 674140000
H	0. 538507000	0. 527098000	-2. 736891000
C	3. 818721000	1. 084396000	-3. 405293000
H	5. 178713000	1. 938435000	-1. 989700000
C	2. 245621000	3. 667477000	0. 404984000
H	2. 138765000	0. 402614000	-4. 648372000
H	4. 578831000	0. 931234000	-4. 168068000
H	1. 926835000	3. 289615000	1. 392172000
H	1. 359148000	3. 602591000	-0. 238142000
C	-2. 791158000	1. 167029000	-0. 403830000
C	-2. 427389000	2. 058720000	0. 591343000
C	-2. 458964000	1. 492104000	-1. 727408000
C	-1. 772856000	3. 258148000	0. 293945000
H	-2. 656551000	1. 848527000	1. 623407000
C	-1. 810240000	2. 669847000	-2. 047181000
H	-2. 730353000	0. 809860000	-2. 520694000
C	-1. 476232000	3. 557375000	-1. 021842000
H	-0. 982525000	4. 488451000	-1. 264274000
C	-3. 644286000	-0. 523970000	1. 374459000
C	-4. 371272000	0. 278497000	2. 266883000
C	-3. 071819000	-1. 681359000	1. 870114000

C	-4.503940000	-0.052209000	3.601268000
H	-4.863290000	1.166731000	1.896656000
C	-3.191771000	-2.041629000	3.216557000
H	-2.548594000	-2.346767000	1.202023000
C	-3.902256000	-1.222500000	4.071352000
H	-4.009818000	-1.494933000	5.112894000
C	-5.104266000	0.075874000	-0.560427000
C	-5.530516000	1.132610000	-1.344689000
C	-6.075970000	-0.830918000	-0.109805000
C	-6.876283000	1.295024000	-1.689977000
H	-4.824419000	1.865072000	-1.702237000
C	-7.410457000	-0.695533000	-0.438109000
H	-5.776218000	-1.660525000	0.514120000
C	-7.804745000	0.380057000	-1.237063000
H	-8.848546000	0.496228000	-1.497114000
C	-1.474671000	3.016519000	-3.496432000
H	-0.400599000	3.124573000	-3.626368000
H	-1.823988000	2.241402000	-4.170624000
H	-1.939442000	3.956540000	-3.784841000
C	-1.434949000	4.232680000	1.421194000
H	-0.873166000	3.736501000	2.207962000
H	-0.843024000	5.062405000	1.050055000
H	-2.343454000	4.634222000	1.865799000
C	-5.306022000	0.830548000	4.555570000
H	-4.677686000	1.196288000	5.364610000
H	-5.722040000	1.685906000	4.033552000
H	-6.124621000	0.270379000	5.001341000
C	-2.539629000	-3.326786000	3.722940000
H	-1.465268000	-3.194428000	3.834915000
H	-2.944734000	-3.612278000	4.688442000
H	-2.702843000	-4.144099000	3.025809000
C	-7.292969000	2.479632000	-2.559850000
H	-8.367636000	2.490913000	-2.709364000
H	-7.001285000	3.419516000	-2.097200000
H	-6.813116000	2.428941000	-3.534644000
C	-8.447971000	-1.702468000	0.054309000
H	-8.878345000	-2.250465000	-0.781172000
H	-7.999907000	-2.418629000	0.735244000
H	-9.260245000	-1.198049000	0.571921000
C	1.872827000	1.513469000	3.255766000
C	1.329321000	1.975226000	4.481711000
C	0.076741000	1.588049000	4.901101000
C	-0.672322000	0.731323000	4.082977000
C	-0.102321000	0.318142000	2.894443000

N	1.130174000	0.672941000	2.463722000
H	-0.321867000	1.944544000	5.847457000
H	1.934673000	2.640261000	5.090384000
H	-1.668777000	0.398504000	4.349957000
H	-0.668844000	-0.332357000	2.233016000
C	3.190804000	1.973160000	2.902002000
H	3.546329000	2.790821000	3.527007000
C	3.989704000	1.552549000	1.882808000
H	4.982618000	1.980741000	1.787518000
H	3.825856000	0.637566000	1.329254000
H	4.343502000	3.254100000	-0.144264000
C	5.615744000	-1.561197000	2.210391000
H	6.056406000	-0.611877000	1.914148000
H	4.707611000	-1.341897000	2.765165000
H	6.312843000	-2.062443000	2.874691000
O	6.693651000	-5.414062000	-0.902616000
O	-4.223590000	-4.055562000	-3.104542000
C	7.877905000	-5.641554000	-0.129389000
H	7.655313000	-5.894673000	0.911557000
H	8.389179000	-6.490631000	-0.587181000
H	8.556009000	-4.783159000	-0.139854000
C	-3.687726000	-5.047439000	-3.988022000
H	-3.121108000	-4.609471000	-4.815160000
H	-3.044833000	-5.765431000	-3.469870000
H	-4.540634000	-5.588004000	-4.402950000

TS2^s_{syn}, $E_{(\text{SCF Done})} = -3313.400566$ a.u. IF = $i164.03$ cm⁻¹

Y	-1.321362000	-0.325804000	0.294066000
N	-1.191833000	-2.871647000	-0.130143000
C	-1.265532000	-3.155192000	-1.577363000
H	-2.319266000	-3.248091000	-1.851518000
H	-0.782550000	-4.116046000	-1.818496000
C	-0.617879000	-2.061269000	-2.418788000
H	0.446889000	-1.977494000	-2.211879000
H	-0.745704000	-2.292039000	-3.484388000
O	-1.183148000	-0.768093000	-2.148281000
C	-2.280961000	-0.437998000	-3.000448000
H	-2.620557000	0.558315000	-2.715272000
H	-3.104674000	-1.148535000	-2.882935000
H	-1.940638000	-0.420609000	-4.042578000
O	0.825691000	-0.722563000	0.149209000
C	1.730725000	-1.647443000	-0.166652000
C	1.358311000	-3.012688000	-0.113722000
C	0.038493000	-3.424076000	0.479050000

H	-0.023218000	-4.525335000	0.447123000
H	0.002599000	-3.150976000	1.541840000
C	3.078922000	-1.340532000	-0.555622000
C	3.918198000	-2.396412000	-0.911546000
H	4.950065000	-2.210126000	-1.177813000
C	3.510699000	-3.736500000	-0.926753000
C	2.221498000	-4.040555000	-0.508204000
H	1.871239000	-5.064277000	-0.452575000
C	3.685950000	0.103516000	-0.344406000
O	-3.343768000	-0.968177000	-0.174287000
C	-4.117226000	-2.028177000	-0.403162000
C	-3.677177000	-3.310816000	0.005932000
C	-2.330212000	-3.455348000	0.645505000
H	-2.309549000	-2.969111000	1.632485000
H	-2.137255000	-4.525882000	0.821094000
C	-5.359294000	-1.944568000	-1.077295000
C	-6.140925000	-3.094463000	-1.260185000
H	-7.087882000	-2.983505000	-1.772767000
C	-5.718140000	-4.344446000	-0.808381000
C	-4.464089000	-4.439892000	-0.190698000
H	-4.115934000	-5.419214000	0.128284000
C	-5.504946000	3.248762000	-0.420983000
H	-6.202640000	2.811953000	-1.153177000
H	-6.138038000	3.593781000	0.410660000
Si	-4.736991000	4.780444000	-1.264448000
C	-3.980540000	6.003642000	-0.026941000
H	-4.726722000	6.328437000	0.708195000
H	-3.142866000	5.555674000	0.517327000
H	-3.611873000	6.897484000	-0.544866000
C	-6.133958000	5.672324000	-2.202114000
H	-6.928527000	5.990286000	-1.516337000
H	-5.758381000	6.567484000	-2.712141000
H	-6.588340000	5.022225000	-2.959320000
C	-3.410418000	4.227715000	-2.509068000
H	-2.588093000	3.716735000	-1.995413000
H	-3.830695000	3.540547000	-3.253999000
H	-2.991059000	5.086470000	-3.046639000
N	-1.504302000	2.102793000	0.375057000
C	-2.364912000	2.751767000	1.269775000
C	-0.259806000	2.626942000	0.217374000
C	-1.786799000	3.672735000	2.210073000
C	-3.743344000	2.540139000	1.276920000
C	0.262986000	3.660804000	0.958937000
H	0.351552000	2.144255000	-0.539393000

C	-0.515994000	4.145584000	2.037819000
H	-2.424707000	4.057428000	3.001163000
C	-4.555304000	2.139834000	0.082397000
H	1.256336000	4.040498000	0.755380000
H	-0.114386000	4.898461000	2.712222000
H	-5.163049000	1.253321000	0.309468000
H	-3.880730000	1.831107000	-0.724388000
C	3.672307000	0.281757000	1.207342000
C	2.917057000	1.224308000	1.879629000
C	4.438269000	-0.613828000	1.970439000
C	2.941907000	1.312665000	3.278003000
H	2.294880000	1.915462000	1.333849000
C	4.479508000	-0.546916000	3.347418000
H	5.017459000	-1.372997000	1.464404000
C	3.726563000	0.434702000	3.997144000
H	3.755772000	0.499588000	5.076680000
C	2.943720000	1.213865000	-1.146997000
C	3.277282000	2.553529000	-0.935630000
C	2.116827000	0.907408000	-2.221832000
C	2.777740000	3.562997000	-1.743834000
H	3.962409000	2.810177000	-0.140430000
C	1.605355000	1.904172000	-3.051541000
H	1.897032000	-0.124967000	-2.448022000
C	1.935186000	3.226890000	-2.799434000
H	1.547578000	4.006553000	-3.441861000
C	5.143563000	0.222799000	-0.912843000
C	6.203451000	0.711126000	-0.170316000
C	5.368365000	-0.058015000	-2.268208000
C	7.471449000	0.887081000	-0.733884000
H	6.065093000	0.973088000	0.867460000
C	6.610787000	0.104200000	-2.848165000
H	4.547546000	-0.409245000	-2.877018000
C	7.666814000	0.576124000	-2.064352000
H	8.643415000	0.707844000	-2.510966000
C	5.336319000	-1.516840000	4.158716000
H	6.139078000	-0.987950000	4.668044000
H	4.740813000	-2.019382000	4.917035000
H	5.780414000	-2.270891000	3.517133000
C	2.112231000	2.381594000	3.986230000
H	1.063112000	2.301330000	3.713152000
H	2.196263000	2.283838000	5.063637000
H	2.449013000	3.377205000	3.706824000
C	3.161209000	5.022525000	-1.506463000
H	3.707808000	5.419087000	-2.359162000

H	2.274300000	5.636036000	-1.367436000
H	3.787165000	5.120271000	-0.625620000
C	0.714320000	1.553073000	-4.241444000
H	-0.294470000	1.931387000	-4.092618000
H	1.101158000	1.996611000	-5.155639000
H	0.659920000	0.478461000	-4.379787000
C	8.613473000	1.420088000	0.129382000
H	9.517112000	1.544725000	-0.458216000
H	8.351842000	2.381963000	0.563889000
H	8.829733000	0.736411000	0.947284000
C	6.840893000	-0.223929000	-4.321987000
H	7.521951000	-1.065851000	-4.426621000
H	5.907190000	-0.479591000	-4.812007000
H	7.280833000	0.623582000	-4.841826000
C	-2.012465000	-0.192331000	3.880309000
C	-1.575199000	-0.407490000	5.215312000
C	-0.349365000	-0.965377000	5.492893000
C	0.492399000	-1.295477000	4.422045000
C	0.031686000	-1.046499000	3.143348000
N	-1.186563000	-0.539129000	2.834676000
H	-0.039075000	-1.132060000	6.521438000
H	-2.247204000	-0.125299000	6.020413000
H	1.486217000	-1.703925000	4.569173000
H	0.686802000	-1.226328000	2.297821000
C	-3.311304000	0.389339000	3.713219000
H	-3.744480000	0.763014000	4.639331000
C	-4.030807000	0.557261000	2.562905000
H	-4.276146000	3.137873000	2.015775000
C	-5.890631000	-0.615972000	-1.627753000
H	-6.589332000	-0.155329000	-0.933112000
H	-5.081878000	0.083554000	-1.799055000
H	-6.414842000	-0.778557000	-2.565299000
H	-5.055940000	0.905856000	2.641042000
H	-3.810895000	0.021310000	1.645872000
O	-6.407330000	-5.587152000	-0.928807000
O	4.520531000	-4.644476000	-1.362896000
C	4.118274000	-6.018217000	-1.309877000
H	3.267095000	-6.230002000	-1.963980000
H	4.971227000	-6.605680000	-1.655039000
H	3.864593000	-6.341142000	-0.295749000
C	-7.703664000	-5.471562000	-1.527730000
H	-7.656478000	-5.112231000	-2.560075000
H	-8.133740000	-6.474997000	-1.532548000
H	-8.368718000	-4.812961000	-0.961429000

TS2^T_{iso}, $E_{(\text{SCF Done})} = -3758.490929 \text{ a.u.}$ IF = $i125.64 \text{ cm}^{-1}$

Y	1.314077000	0.025247000	0.328391000
N	1.592588000	-2.303862000	-0.859510000
C	1.487512000	-3.425227000	0.095119000
H	2.492738000	-3.650294000	0.462747000
H	1.111228000	-4.334217000	-0.401407000
C	0.584923000	-3.089915000	1.269610000
H	-0.434199000	-2.901446000	0.938255000
H	0.569139000	-3.921666000	1.986279000
O	1.016958000	-1.895802000	1.934349000
C	1.977149000	-2.119193000	2.967060000
H	2.186256000	-1.148482000	3.417681000
H	2.906408000	-2.539782000	2.568751000
H	1.553652000	-2.790737000	3.724193000
O	-0.712134000	-0.499449000	-0.246092000
C	-1.485830000	-1.395816000	-0.823412000
C	-0.880150000	-2.440870000	-1.584742000
C	0.583278000	-2.409336000	-1.942973000
H	0.803076000	-3.318128000	-2.529445000
H	0.779874000	-1.563818000	-2.613357000
C	-2.918423000	-1.362530000	-0.713533000
C	-3.643878000	-2.392717000	-1.315312000
H	-4.725838000	-2.385957000	-1.265767000
C	-3.038212000	-3.439224000	-2.007622000
C	-1.655302000	-3.452568000	-2.142466000
H	-1.176623000	-4.245726000	-2.716018000
C	-3.648793000	-0.182741000	0.048535000
O	3.391270000	-0.526753000	0.586915000
C	4.298536000	-1.461180000	0.392636000
C	4.118034000	-2.409842000	-0.645546000
C	2.923395000	-2.295822000	-1.545323000
H	2.965500000	-1.361801000	-2.122863000
H	2.953926000	-3.121628000	-2.275852000
C	5.455800000	-1.552167000	1.216985000
C	6.379912000	-2.567352000	0.978772000
H	7.266945000	-2.634949000	1.605728000
C	6.199928000	-3.495680000	-0.049290000
C	5.063794000	-3.412552000	-0.851331000
H	4.917954000	-4.133710000	-1.654905000
C	2.147315000	5.621270000	0.129036000
H	1.327183000	6.131843000	0.656549000
H	3.031135000	5.758157000	0.771156000
Si	2.432229000	6.611421000	-1.481427000

C	4.038670000	6.132219000	-2.377759000
H	4.905146000	6.203353000	-1.709313000
H	3.991081000	5.109083000	-2.765156000
H	4.216833000	6.806234000	-3.224730000
C	2.548110000	8.448435000	-0.996462000
H	3.385866000	8.626398000	-0.311485000
H	2.701430000	9.079282000	-1.880198000
H	1.632128000	8.788065000	-0.498563000
C	0.969831000	6.379925000	-2.670025000
H	0.874415000	5.333956000	-2.982069000
H	0.024733000	6.682960000	-2.204370000
H	1.105187000	6.986702000	-3.573339000
N	1.651528000	1.552418000	-1.482719000
C	2.833888000	2.294921000	-1.427215000
C	1.330295000	0.962659000	-2.667465000
C	3.841945000	2.013636000	-2.414240000
C	2.983089000	3.312528000	-0.481178000
C	2.188823000	0.854720000	-3.736144000
H	0.326411000	0.543620000	-2.707049000
C	3.517219000	1.330373000	-3.554616000
H	4.833319000	2.438811000	-2.279829000
C	1.821117000	4.118913000	0.031200000
H	1.870764000	0.386110000	-4.661584000
H	4.262013000	1.180412000	-4.332846000
H	1.508322000	3.787382000	1.035811000
H	0.953215000	3.953252000	-0.619306000
C	-2.960265000	1.157823000	-0.366674000
C	-2.651592000	2.171575000	0.525227000
C	-2.690868000	1.377444000	-1.725620000
C	-2.115259000	3.388014000	0.091571000
H	-2.834945000	2.045696000	1.579908000
C	-2.157835000	2.569401000	-2.179251000
H	-2.920905000	0.599662000	-2.440168000
C	-1.879691000	3.579943000	-1.256419000
H	-1.478396000	4.522070000	-1.604239000
C	-3.621761000	-0.414054000	1.594634000
C	-4.391492000	0.413491000	2.425910000
C	-2.947263000	-1.468572000	2.183231000
C	-4.466666000	0.208274000	3.789841000
H	-4.962951000	1.218388000	1.985850000
C	-3.007554000	-1.701400000	3.561239000
H	-2.389063000	-2.156024000	1.567900000
C	-3.761892000	-0.858516000	4.353284000
H	-3.823727000	-1.033531000	5.419208000

C	-5.171515000	-0.137629000	-0.341839000
C	-5.710183000	0.801487000	-1.202673000
C	-6.045993000	-1.080175000	0.220604000
C	-7.073667000	0.814238000	-1.515200000
H	-5.081888000	1.556682000	-1.647521000
C	-7.395320000	-1.091875000	-0.073019000
H	-5.657454000	-1.818498000	0.907173000
C	-7.904469000	-0.132416000	-0.951148000
H	-8.960925000	-0.131378000	-1.184777000
C	-1.891105000	2.798747000	-3.665692000
H	-0.836937000	3.000050000	-3.840124000
H	-2.173947000	1.928456000	-4.248749000
H	-2.456121000	3.653529000	-4.030365000
C	-1.841338000	4.496337000	1.107017000
H	-1.240700000	4.126257000	1.933378000
H	-1.313837000	5.323164000	0.643751000
H	-2.774063000	4.876088000	1.519599000
C	-5.315471000	1.116469000	4.677512000
H	-4.699252000	1.613350000	5.423523000
H	-5.815507000	1.876893000	4.086825000
H	-6.071879000	0.540367000	5.205235000
C	-2.243760000	-2.875028000	4.171682000
H	-1.186855000	-2.635557000	4.271740000
H	-2.627106000	-3.115232000	5.158198000
H	-2.326966000	-3.758864000	3.545338000
C	-7.617224000	1.873656000	-2.472121000
H	-8.692851000	1.781305000	-2.580960000
H	-7.393904000	2.873503000	-2.107560000
H	-7.164479000	1.772248000	-3.455893000
C	-8.326121000	-2.134163000	0.543464000
H	-8.734901000	-2.786728000	-0.225010000
H	-7.796698000	-2.748273000	1.264508000
H	-9.161292000	-1.654766000	1.048263000
C	1.715834000	2.295208000	3.086033000
C	1.160481000	2.837508000	4.275728000
C	-0.034403000	2.382013000	4.781613000
C	-0.718787000	1.369967000	4.090735000
C	-0.143601000	0.881823000	2.935358000
N	1.037322000	1.301113000	2.420824000
H	-0.440222000	2.802501000	5.698299000
H	1.713907000	3.620997000	4.784940000
H	-1.670165000	0.977020000	4.430647000
H	-0.661488000	0.109886000	2.371185000
C	2.966252000	2.836583000	2.633277000

H	3.253418000	3.752917000	3.146390000
C	3.774583000	2.385780000	1.627507000
H	4.723832000	2.886668000	1.464618000
H	3.709764000	1.387665000	1.215655000
H	3.934444000	3.836849000	-0.537372000
C	5.683350000	-0.530140000	2.334782000
H	6.013597000	0.423472000	1.929060000
H	4.768207000	-0.350037000	2.892526000
H	6.443542000	-0.883784000	3.024350000
C	-3.904555000	-4.591733000	-2.611157000
C	7.236624000	-4.645699000	-0.266404000
F	-3.323830000	-5.121833000	-3.739040000
F	-4.063150000	-5.628140000	-1.716173000
F	-5.162697000	-4.157260000	-2.951937000
F	7.268976000	-5.055705000	-1.577909000
F	8.507080000	-4.255491000	0.083205000
F	6.930706000	-5.753568000	0.494765000

TS2^T_{syn}, $E_{(\text{SCF Done})} = -3758.479392$ a.u. IF = $i180.26$ cm⁻¹

Y	1.286933000	-0.065610000	0.353175000
N	1.294253000	2.502867000	0.126295000
C	1.377999000	2.899722000	-1.293823000
H	2.433921000	2.958434000	-1.568646000
H	0.946097000	3.901038000	-1.452798000
C	0.668969000	1.912326000	-2.213278000
H	-0.400218000	1.880037000	-2.014476000
H	0.816384000	2.210032000	-3.259340000
O	1.154438000	0.571176000	-2.033559000
C	2.208223000	0.218071000	-2.931863000
H	2.489410000	-0.811608000	-2.707177000
H	3.077692000	0.868929000	-2.799398000
H	1.843055000	0.278306000	-3.963643000
O	-0.856894000	0.448699000	0.252720000
C	-1.702717000	1.439012000	0.026671000
C	-1.243332000	2.781887000	0.182896000
C	0.099861000	3.072922000	0.789596000
H	0.218460000	4.168773000	0.839075000
H	0.129992000	2.719794000	1.828647000
C	-3.073391000	1.236308000	-0.361711000
C	-3.857581000	2.364440000	-0.617155000
H	-4.902750000	2.237638000	-0.872464000
C	-3.370010000	3.666198000	-0.533763000
C	-2.060140000	3.866335000	-0.119922000
H	-1.678776000	4.879772000	-0.000458000

C	-3.745727000	-0.189861000	-0.262777000
O	3.349627000	0.507916000	-0.099311000
C	4.172157000	1.532903000	-0.243428000
C	3.800628000	2.800672000	0.279171000
C	2.466416000	2.958871000	0.938746000
H	2.420974000	2.395694000	1.883306000
H	2.330951000	4.019810000	1.203407000
C	5.411916000	1.432395000	-0.939369000
C	6.240646000	2.552700000	-1.020657000
H	7.192227000	2.463464000	-1.541327000
C	5.886835000	3.778180000	-0.458563000
C	4.651311000	3.897324000	0.172461000
H	4.347515000	4.857453000	0.587675000
C	5.312312000	-3.755785000	-0.624533000
H	6.031963000	-3.300168000	-1.323081000
H	5.924030000	-4.163435000	0.194689000
Si	4.514394000	-5.216441000	-1.562176000
C	3.732800000	-6.496264000	-0.399796000
H	4.470789000	-6.871889000	0.319170000
H	2.898350000	-6.067031000	0.163916000
H	3.354093000	-7.354463000	-0.968315000
C	5.896183000	-6.076034000	-2.550837000
H	6.682630000	-6.451422000	-1.885040000
H	5.504441000	-6.929876000	-3.116532000
H	6.365075000	-5.388683000	-3.265115000
C	3.203626000	-4.562677000	-2.773528000
H	2.391999000	-4.060095000	-2.235484000
H	3.642463000	-3.846662000	-3.479497000
H	2.766620000	-5.381621000	-3.357025000
N	1.341888000	-2.478145000	0.171733000
C	2.150378000	-3.245578000	1.020607000
C	0.086507000	-2.939972000	-0.080658000
C	1.510165000	-4.231652000	1.847242000
C	3.536606000	-3.092046000	1.077514000
C	-0.491989000	-4.023850000	0.535156000
H	-0.481260000	-2.362398000	-0.804475000
C	0.232486000	-4.640717000	1.585474000
H	2.107516000	-4.715476000	2.615287000
C	4.388593000	-2.647539000	-0.075009000
H	-1.488300000	-4.347983000	0.262058000
H	-0.216427000	-5.443594000	2.165613000
H	5.017898000	-1.795365000	0.214506000
H	3.740992000	-2.272294000	-0.876183000
C	-3.692878000	-0.522863000	1.262539000

C	-2.988959000	-1.578896000	1.810749000
C	-4.370491000	0.341112000	2.137423000
C	-2.981706000	-1.806983000	3.193550000
H	-2.434517000	-2.253128000	1.177385000
C	-4.379543000	0.137020000	3.501493000
H	-4.908673000	1.185157000	1.730156000
C	-3.681751000	-0.955347000	4.023314000
H	-3.686576000	-1.128482000	5.091234000
C	-3.086721000	-1.249506000	-1.196657000
C	-3.496519000	-2.582399000	-1.117404000
C	-2.263742000	-0.880319000	-2.254442000
C	-3.076007000	-3.528148000	-2.039597000
H	-4.180410000	-2.881101000	-0.335883000
C	-1.830998000	-1.811751000	-3.197190000
H	-1.986073000	0.155455000	-2.378104000
C	-2.235817000	-3.132043000	-3.076209000
H	-1.909813000	-3.860535000	-3.806881000
C	-5.225812000	-0.180316000	-0.785049000
C	-6.290385000	-0.661750000	-0.045116000
C	-5.475192000	0.222263000	-2.105172000
C	-7.584210000	-0.714764000	-0.574467000
H	-6.136833000	-1.014460000	0.963157000
C	-6.742811000	0.182917000	-2.650715000
H	-4.653329000	0.570352000	-2.714429000
C	-7.801322000	-0.286120000	-1.868297000
H	-8.797904000	-0.321921000	-2.287999000
C	-5.145915000	1.073347000	4.433720000
H	-5.994313000	0.560004000	4.881449000
H	-4.508991000	1.422713000	5.242519000
H	-5.519386000	1.937316000	3.893739000
C	-2.209853000	-2.994999000	3.763869000
H	-1.155195000	-2.930346000	3.507760000
H	-2.299343000	-3.029583000	4.844684000
H	-2.589436000	-3.930201000	3.359373000
C	-3.547632000	-4.978346000	-1.948756000
H	-4.181888000	-5.228406000	-2.796501000
H	-2.701133000	-5.660471000	-1.956197000
H	-4.115396000	-5.144995000	-1.039266000
C	-0.945619000	-1.389227000	-4.367965000
H	0.035893000	-1.852262000	-4.296261000
H	-1.386287000	-1.696207000	-5.313342000
H	-0.816157000	-0.312268000	-4.386117000
C	-8.729916000	-1.245225000	0.285432000
H	-9.656684000	-1.271322000	-0.278264000

H	-8.514036000	-2.251230000	0.637213000
H	-8.879438000	-0.614864000	1.159192000
C	-6.998051000	0.642152000	-4.084843000
H	-7.632962000	1.525496000	-4.098306000
H	-6.066540000	0.885529000	-4.585195000
H	-7.501148000	-0.135132000	-4.654715000
C	1.966269000	-0.511446000	3.906810000
C	1.542813000	-0.378658000	5.256963000
C	0.351023000	0.223951000	5.583848000
C	-0.472183000	0.683141000	4.545867000
C	-0.028213000	0.509612000	3.249753000
N	1.160614000	-0.038395000	2.894845000
H	0.051450000	0.327333000	6.623858000
H	2.199159000	-0.760654000	6.033408000
H	-1.440896000	1.134622000	4.729938000
H	-0.674035000	0.790848000	2.425487000
C	3.229070000	-1.148593000	3.685310000
H	3.642920000	-1.624327000	4.572575000
C	3.932841000	-1.257118000	2.517548000
H	4.023821000	-3.775973000	1.771654000
C	5.864478000	0.127786000	-1.603563000
H	6.521080000	-0.439549000	-0.947991000
H	5.015390000	-0.498971000	-1.847611000
H	6.412823000	0.341982000	-2.516550000
H	4.938694000	-1.663477000	2.555696000
H	3.744153000	-0.623251000	1.657756000
C	-4.287506000	4.879154000	-0.894536000
C	6.828609000	5.018413000	-0.596919000
F	-3.920290000	6.010539000	-0.205143000
F	-5.606004000	4.621637000	-0.605491000
F	-4.219100000	5.184849000	-2.236566000
F	8.151417000	4.648026000	-0.631209000
F	6.664369000	5.894484000	0.449565000
F	6.574847000	5.721298000	-1.755013000

TS2^u_{iso}, $E_{\text{(SCF Done)}} = -3084.445131$ a.u. IF = $i102.18$ cm⁻¹

Y	1.343504000	-0.915463000	0.016528000
N	1.203176000	-2.858867000	-1.737325000
C	0.781538000	-4.130396000	-1.118701000
H	1.681886000	-4.665595000	-0.803216000
H	0.259049000	-4.771306000	-1.847353000
C	-0.121467000	-3.908780000	0.082700000
H	-1.043490000	-3.410141000	-0.208722000
H	-0.378103000	-4.870277000	0.547117000

O	0.500001000	-3.061010000	1.057027000
C	1.306116000	-3.761164000	2.004173000
H	1.677880000	-3.019988000	2.712340000
H	2.155570000	-4.257367000	1.523287000
H	0.691254000	-4.497958000	2.536232000
O	-0.689646000	-0.788320000	-0.714916000
C	-1.597476000	-1.309246000	-1.526494000
C	-1.174985000	-2.235199000	-2.521323000
C	0.284487000	-2.445810000	-2.827247000
H	0.352938000	-3.194914000	-3.634939000
H	0.710988000	-1.522016000	-3.237105000
C	-2.989358000	-0.979254000	-1.442743000
C	-3.870863000	-1.630774000	-2.313582000
H	-4.924220000	-1.386263000	-2.276198000
C	-3.457088000	-2.577655000	-3.244764000
C	-2.104255000	-2.867353000	-3.346783000
H	-1.751927000	-3.576363000	-4.094545000
C	-3.509696000	0.104025000	-0.411872000
O	3.214281000	-1.975572000	0.161231000
C	3.913324000	-3.019574000	-0.255682000
C	3.618866000	-3.599056000	-1.511247000
C	2.554965000	-2.983598000	-2.369808000
H	2.845732000	-1.968427000	-2.674692000
H	2.461173000	-3.576787000	-3.295087000
C	4.944527000	-3.587308000	0.537932000
C	5.642538000	-4.695728000	0.053008000
H	6.431242000	-5.122981000	0.668312000
C	5.354985000	-5.262463000	-1.187898000
C	4.338379000	-4.709183000	-1.959508000
H	4.095073000	-5.139374000	-2.929809000
C	3.394938000	4.218596000	1.334910000
H	2.666800000	4.758297000	1.959607000
H	4.243268000	4.002750000	2.003029000
Si	3.992833000	5.469002000	0.019659000
C	5.548106000	4.892696000	-0.908633000
H	6.349983000	4.615899000	-0.213665000
H	5.334794000	4.026410000	-1.543605000
H	5.927620000	5.697061000	-1.550747000
C	4.413628000	7.082471000	0.938875000
H	5.201565000	6.919610000	1.684103000
H	4.767855000	7.853205000	0.243981000
H	3.537105000	7.482115000	1.462655000
C	2.618416000	5.816111000	-1.242926000
H	2.332900000	4.899906000	-1.771882000

H	1.722531000	6.222141000	-0.758824000
H	2.951444000	6.544485000	-1.991881000
N	2.171751000	0.915428000	-1.298312000
C	3.478389000	1.318347000	-1.008310000
C	1.843535000	0.730098000	-2.605924000
C	4.488505000	1.060926000	-2.000890000
C	3.761785000	1.998063000	0.177410000
C	2.753828000	0.691224000	-3.636827000
H	0.780752000	0.580271000	-2.789359000
C	4.130864000	0.779566000	-3.291147000
H	5.531970000	1.190241000	-1.725022000
C	2.768196000	2.889884000	0.867967000
H	2.428841000	0.553844000	-4.662759000
H	4.894941000	0.655054000	-4.055112000
H	2.335205000	2.405496000	1.760252000
H	1.923404000	3.077541000	0.193291000
C	-2.514543000	1.309390000	-0.432308000
C	-2.076413000	1.964249000	0.706700000
C	-2.083076000	1.798168000	-1.674456000
C	-1.252411000	3.091464000	0.630341000
H	-2.376410000	1.621127000	1.683436000
C	-1.267090000	2.909000000	-1.776729000
H	-2.409064000	1.300905000	-2.577144000
C	-0.860921000	3.559133000	-0.609368000
H	-0.235420000	4.438409000	-0.680357000
C	-3.668752000	-0.512616000	1.016191000
C	-4.314149000	0.227869000	2.018089000
C	-3.286718000	-1.807158000	1.318795000
C	-4.549494000	-0.296323000	3.274187000
H	-4.660800000	1.226988000	1.795201000
C	-3.514055000	-2.364019000	2.581670000
H	-2.834524000	-2.421588000	0.556637000
C	-4.138766000	-1.603010000	3.549852000
H	-4.328346000	-2.025518000	4.527680000
C	-4.946067000	0.601735000	-0.816388000
C	-5.188041000	1.822510000	-1.420229000
C	-6.053360000	-0.215975000	-0.541546000
C	-6.482528000	2.232490000	-1.756757000
H	-4.372346000	2.493436000	-1.637936000
C	-7.341006000	0.163117000	-0.865437000
H	-5.898669000	-1.170718000	-0.059979000
C	-7.547841000	1.400390000	-1.479632000
H	-8.553533000	1.707487000	-1.734378000
C	-0.824121000	3.438957000	-3.139121000

H	0.259332000	3.413913000	-3.226980000
H	-1.245612000	2.843031000	-3.941983000
H	-1.143476000	4.469873000	-3.273531000
C	-0.834895000	3.809079000	1.913040000
H	-0.395072000	3.112768000	2.621840000
H	-0.108499000	4.586490000	1.701936000
H	-1.696700000	4.269378000	2.392413000
C	-5.259886000	0.523698000	4.349473000
H	-4.618350000	0.662523000	5.216845000
H	-5.536462000	1.501863000	3.970115000
H	-6.162732000	0.018695000	4.684717000
C	-3.070981000	-3.796078000	2.875437000
H	-1.998650000	-3.837102000	3.056564000
H	-3.574163000	-4.184518000	3.755113000
H	-3.291526000	-4.449423000	2.035832000
C	-6.692969000	3.591529000	-2.421862000
H	-7.747643000	3.778355000	-2.595501000
H	-6.301589000	4.391116000	-1.797315000
H	-6.176012000	3.636650000	-3.377733000
C	-8.529538000	-0.747085000	-0.562192000
H	-9.036279000	-1.037583000	-1.479816000
H	-8.206944000	-1.648344000	-0.051322000
H	-9.254723000	-0.237384000	0.067766000
C	1.984693000	0.402540000	3.314183000
C	1.457206000	0.733510000	4.589764000
C	0.147563000	0.465344000	4.915412000
C	-0.677339000	-0.134733000	3.952990000
C	-0.119484000	-0.429221000	2.724661000
N	1.167210000	-0.188045000	2.381176000
H	-0.237837000	0.718010000	5.899922000
H	2.121859000	1.199358000	5.311226000
H	-1.720178000	-0.361374000	4.142782000
H	-0.741163000	-0.879251000	1.954622000
C	3.363322000	0.723982000	3.063325000
H	3.800974000	1.376963000	3.816700000
C	4.136916000	0.364591000	1.998503000
H	5.183494000	0.653001000	1.997470000
H	3.880312000	-0.434737000	1.315766000
H	4.808650000	2.266946000	0.301453000
C	5.295616000	-2.974336000	1.897188000
H	5.865781000	-2.056068000	1.775600000
H	4.399307000	-2.730621000	2.461260000
H	5.893559000	-3.665330000	2.483354000
H	-4.181658000	-3.061814000	-3.893402000

H	5.913069000	-6.123803000	-1.544553000
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TS2^u_{sym}, $E_{\text{(SCF Done)}} = -3084.433091$ a.u. IF = $i168.52$ cm⁻¹

Y	-1.365067000	-0.775792000	-0.007964000
N	-1.077889000	-3.093113000	-1.102777000
C	-1.119763000	-2.980032000	-2.574104000
H	-2.163714000	-3.053299000	-2.889080000
H	-0.576760000	-3.811432000	-3.052163000
C	-0.530691000	-1.665413000	-3.072248000
H	0.526370000	-1.584714000	-2.827794000
H	-0.639023000	-1.601754000	-4.162766000
O	-1.171308000	-0.528059000	-2.471038000
C	-2.275376000	-0.029824000	-3.228459000
H	-2.677576000	0.825874000	-2.684925000
H	-3.056612000	-0.787681000	-3.339725000
H	-1.922805000	0.298742000	-4.213215000
O	0.809667000	-0.989797000	-0.194594000
C	1.771059000	-1.739771000	-0.723452000
C	1.474527000	-3.092312000	-1.053307000
C	0.176728000	-3.721068000	-0.631585000
H	0.185413000	-4.773390000	-0.963865000
H	0.108751000	-3.752823000	0.463793000
C	3.099469000	-1.262002000	-0.977208000
C	4.010541000	-2.139245000	-1.580609000
H	5.026332000	-1.803659000	-1.745479000
C	3.685133000	-3.435173000	-1.964781000
C	2.413127000	-3.908640000	-1.682822000
H	2.142089000	-4.934211000	-1.928249000
C	3.606577000	0.105619000	-0.369981000
O	-3.341805000	-1.376375000	-0.693085000
C	-4.046494000	-2.371361000	-1.221978000
C	-3.533811000	-3.690486000	-1.160179000
C	-2.190923000	-3.923047000	-0.541513000
H	-2.209628000	-3.714889000	0.539296000
H	-1.934246000	-4.989243000	-0.648485000
C	-5.284711000	-2.166474000	-1.888115000
C	-5.977582000	-3.271018000	-2.395842000
H	-6.927982000	-3.095853000	-2.895100000
C	-5.487943000	-4.569249000	-2.291038000
C	-4.252015000	-4.765485000	-1.684886000
H	-3.828324000	-5.766193000	-1.618716000
C	-5.758754000	2.610746000	0.172421000
H	-6.419913000	2.355875000	-0.671043000
H	-6.421044000	2.678652000	1.048875000

Si	-5.069644000	4.353885000	-0.195836000
C	-4.426314000	5.234765000	1.357225000
H	-5.206771000	5.297026000	2.125137000
H	-3.569090000	4.706938000	1.787515000
H	-4.111912000	6.258030000	1.118077000
C	-6.496849000	5.385713000	-0.920037000
H	-7.333662000	5.451693000	-0.214296000
H	-6.171768000	6.408178000	-1.146570000
H	-6.877680000	4.942362000	-1.847836000
C	-3.677910000	4.232021000	-1.484484000
H	-2.847653000	3.629265000	-1.098925000
H	-4.039115000	3.767999000	-2.410822000
H	-3.286889000	5.224249000	-1.738869000
N	-1.705228000	1.523501000	0.718569000
C	-2.610913000	1.851440000	1.736027000
C	-0.497987000	2.148812000	0.734269000
C	-2.099033000	2.519215000	2.901678000
C	-3.972865000	1.561498000	1.654566000
C	-0.048856000	2.976025000	1.737041000
H	0.146914000	1.927599000	-0.111183000
C	-0.862480000	3.101377000	2.889736000
H	-2.763994000	2.634773000	3.753274000
C	-4.750864000	1.458804000	0.377305000
H	0.917237000	3.459420000	1.664372000
H	-0.514795000	3.669048000	3.749816000
H	-5.307365000	0.512534000	0.339649000
H	-4.053228000	1.419740000	-0.466984000
C	3.565635000	-0.137012000	1.172584000
C	2.742674000	0.543297000	2.050497000
C	4.381414000	-1.155281000	1.691210000
C	2.747320000	0.256099000	3.422201000
H	2.081506000	1.315717000	1.691463000
C	4.404421000	-1.456176000	3.036940000
H	5.014474000	-1.715094000	1.017691000
C	3.581344000	-0.731980000	3.903423000
H	3.595240000	-0.956170000	4.961709000
C	2.803527000	1.345283000	-0.867765000
C	3.046247000	2.596577000	-0.296739000
C	2.012751000	1.290319000	-2.010051000
C	2.493170000	3.754583000	-0.821175000
H	3.702485000	2.670791000	0.558495000
C	1.449390000	2.441135000	-2.559300000
H	1.863950000	0.345123000	-2.509810000
C	1.688966000	3.664909000	-1.953506000

H	1. 260564000	4. 564046000	-2. 376407000
C	5. 059220000	0. 462800000	-0. 844809000
C	6. 076673000	0. 798979000	0. 029735000
C	5. 316385000	0. 570504000	-2. 219404000
C	7. 335508000	1. 198678000	-0. 431175000
H	5. 910957000	0. 763585000	1. 095582000
C	6. 550421000	0. 959794000	-2. 700452000
H	4. 526956000	0. 345176000	-2. 922120000
C	7. 564594000	1. 269138000	-1. 790293000
H	8. 534336000	1. 576716000	-2. 158454000
C	5. 316123000	-2. 552535000	3. 584546000
H	6. 081646000	-2. 129196000	4. 231383000
H	4. 749467000	-3. 270595000	4. 172279000
H	5. 809871000	-3. 084409000	2. 777853000
C	1. 840793000	1. 043422000	4. 366065000
H	0. 801366000	0. 968407000	4. 056734000
H	1. 925524000	0. 671188000	5. 381783000
H	2. 108229000	2. 097529000	4. 365602000
C	2. 778065000	5. 117072000	-0. 191784000
H	3. 313618000	5. 757328000	-0. 889223000
H	1. 851375000	5. 619820000	0. 074272000
H	3. 380398000	5. 011527000	0. 704495000
C	0. 601443000	2. 370755000	-3. 827810000
H	-0. 429608000	2. 646316000	-3. 618449000
H	0. 979452000	3. 057312000	-4. 581440000
H	0. 610529000	1. 368877000	-4. 243753000
C	8. 429798000	1. 552092000	0. 574417000
H	9. 333237000	1. 873170000	0. 066404000
H	8. 103705000	2. 353859000	1. 232731000
H	8. 674093000	0. 693639000	1. 196046000
C	6. 815718000	1. 059094000	-4. 201356000
H	7. 594211000	0. 361367000	-4. 502040000
H	5. 918797000	0. 833916000	-4. 768901000
H	7. 147975000	2. 059411000	-4. 468580000
C	-2. 094723000	-1. 671506000	3. 458495000
C	-1. 657022000	-2. 218777000	4. 694919000
C	-0. 399426000	-2. 755141000	4. 842388000
C	0. 472985000	-2. 724230000	3. 745977000
C	0. 008925000	-2. 162001000	2. 572214000
N	-1. 237579000	-1. 665551000	2. 380923000
H	-0. 088569000	-3. 179423000	5. 793880000
H	-2. 354224000	-2. 210873000	5. 527583000
H	1. 490604000	-3. 094869000	3. 802907000
H	0. 682423000	-2. 061397000	1. 728161000

C	-3.426978000	-1.146075000	3.420903000
H	-3.894649000	-1.069947000	4.400885000
C	-4.141591000	-0.708976000	2.340016000
H	-4.546500000	1.902093000	2.516062000
C	-5.886078000	-0.768907000	-2.070291000
H	-6.608908000	-0.546982000	-1.288555000
H	-5.117448000	-0.006526000	-2.037774000
H	-6.401074000	-0.702568000	-3.024550000
H	-5.188671000	-0.458703000	2.479630000
H	-3.876459000	-0.958059000	1.318174000
H	-6.049393000	-5.408561000	-2.691877000
H	4.425737000	-4.069086000	-2.444097000