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Supplementary Information

Theoretical mechanistic insights into dinitrogen cleavage by a dititanium hydride complex bearing PNP-pincer ligands

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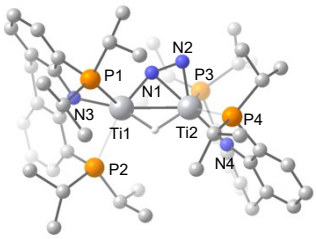
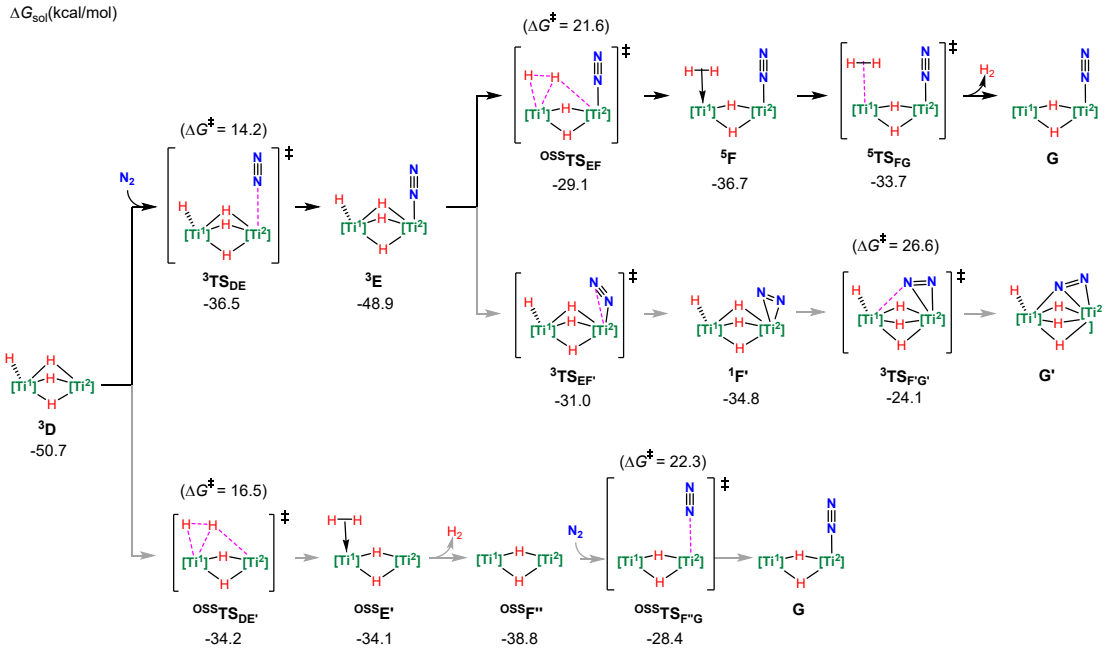
Tab. S1 Selected important bond distances (Å) in the DFTs-optimized complex **¹2m** and corresponding X-ray data and the unsigned errors (|Δ|) of the corresponding DFT-optimized bond distances in comparison with the X-ray data.



2m

Bond	X-ray data	TPSSTPSS		TPSSTPSS-D3(BJ)		BP86		BP86-D3(BJ)	
		distance	|Δ|	distance	|Δ|	distance	|Δ|	distance	|Δ|
Ti1–Ti2	2.703	2.686	0.017	2.644	0.059	2.698	0.005	2.639	0.064
Ti1–N1	1.845	1.840	0.005	1.848	0.003	1.834	0.011	1.845	0.000
Ti2–N2	1.904	1.879	0.025	1.882	0.022	1.874	0.030	1.877	0.027
N1–N2	1.297	1.306	0.009	1.308	0.011	1.306	0.009	1.309	0.012
Ti1–N3	2.086	2.079	0.007	2.072	0.014	2.081	0.005	2.074	0.012
Ti1–N4	2.203	2.216	0.013	2.198	0.005	2.227	0.024	2.206	0.003
Ti1–P1	2.582	2.617	0.035	2.542	0.040	2.618	0.036	2.521	0.061
Ti1–P2	2.678	2.662	0.016	2.575	0.103	2.672	0.006	2.556	0.122
Ti2–P3	2.550	2.569	0.019	2.511	0.039	2.570	0.020	2.498	0.052
Ti2–P4	2.613	2.621	0.008	2.565	0.048	2.613	0.000	2.541	0.072
Average error			**0.015**		**0.034**		**0.015**		**0.043**

Scheme S1 The calculated free energy profile for the transformation of **³D**.



For transformation of tetrahydride intermediate ^{3}**D**, the H_2 elimination prior to N_2 coordination is less favorable both thermodynamically and dynamically. For transformation of ^{3}**D**, the direct H_2 elimination is more favorable than β-N of N_2 ligand coordination to the other Ti centre (Scheme S1).

Tab. S2 Energy profile for Ti(III) and Ti(II) species at various electronic states (energies in kcal mol^{-1}). The numbers in bold represent the energies of the more favorable spin state.[a]

(a) Transformation from **1m** to **2m** (Gibbs free energies relative to **1m**)

species	closed-shell singlet	open-shell singlet	triplet	quintet[b]
C	–34.5	–37.5	**–39.9**	
TS$_{CD}$	–31.2	–36.8	**–37.5**	
D	–37.1	–48.3	**–50.7**	
TS$_{DE}$	–26.6	–32.2	**–36.6**	
E	–41.0	–45.0	**–48.9**	
TS$_{EF}$	*	**–29.1**	*	–12.7
F	*	–35.7	–32.1	**–36.7**
TS$_{FG}$	*	–32.9	–29.2	**–33.7**
G	*	**–43.5**	–39.8	–43.0
TS$_{G2m'}$	*	–39.3	–37.0	**–39.4**
2m'	**–51.6**	**	–50.3	–37.3
TS$_{DE'}$	*	**–34.2**	*	–12.6
E'	*	**–34.1**	*	–33.3
TS$_{EF'}$	–22.9	–28.0	**–31.0**	
F'	**–34.8**	**	–33.8	
TS$_{F'G'}$	–23.1	**	**–24.1**	
F''	–24.7	**–38.8**	–30.8	–38.6
TS$_{F''G}$	–11.9	**–28.4**	–22.2	–27.9

(b) Transformation from **2m** to **5m** (Gibbs free energies relative to **2m**).

species	closed-shell singlet	open-shell singlet	triplet
2m	**0.0**	**	3.2
TS$_{IJ}$	**22.2**	**	24.1
J	23.0	20.7	**17.0**
TS$_{JK}$	32.0	23.7	**21.5**
K	19.0	12.8	**12.1**
TS$_{K5m}$	27.3	24.7	**21.3**
TS$_{[2m-1]}$	42.3	38.3	**35.2**
TS$_{[2m-2]}$	37.1	35.1	**34.6**
TS$_{[2m-3]}$	44.2	42.4	**39.3**
TS$_{[H'-1]}$	36.0	**	**28.1**
TS$_{[H'-2]}$	38.6	34.2	**33.8**

[a] * denotes the structure failed to locate, ** denotes the open-shell singlet converged to closed-shell singlet.

[b] Quintet is only considered for Ti(II) species.

Tab. S3 Imaginary frequency of transition states (*IF*, cm^{-1}), Gas-phase thermal corrections to Gibbs free energy ($\Delta\Delta G_{gas}$, a.u.), and single-point energy (E_{sp}, a.u.) in solution.

(a) Transformation from **1m** to **2m**, and **2m** to **5m** at TPSSTPSS/BSII//TPSSTPSS/BSI level

species	$\Delta\Delta G_{gas}$	E_{sp}	species	$\Delta\Delta G_{gas}$	E_{sp}	*IF*
H_2	−0.001306	−1.179614	^{2}**TS$_{1mA}$**	0.564031	−2643.021491	691.73i
N_2	−0.013056	−109.588346	^{2}**TS$_{AB}$**	0.537961	−2603.685163	1166.49i
^{2}**1m**	0.548339	−2641.857428S	^{1}**TS$_{CD}$**	1.024921	−5126.399533	359.02i
methane	0.027661	−40.540226	^{OSS}**TS$_{CD}$**	1.022140	−5126.405624	171.39i
^{2}**A**	0.521064	−2602.520697	^{3}**TS$_{CD}$**	1.022230	−5126.406769	361.93i
^{2}**B**	0.495303	−2563.174353	^{1}**TS$_{DE}$**	1.030389	−5235.999049	46.79i
^{1}**C**	1.025939	−5126.405792	^{OSS}**TS$_{DE}$**	1.028561	−5236.006179	83.43i
^{OSS}**C**	1.022107	−5126.406709	^{3}**TS$_{DE}$**	1.027340	−5236.011868	48.47i
^{3}**C**	1.022456	−5126.410906	^{OSS}**TS$_{EF}$**	1.030276	−5236.002821	865.12i
^{1}**D**	1.026631	−5126.410587	^{5}**TS$_{EF}$**	1.026904	−5235.973461	853.78i
^{OSS}**D**	1.025778	−5126.427651	^{OSS}**TS$_{FG}$**	1.026152	−5236.004864	106.93i
^{3}**D**	1.025136	−5126.430798	^{3}**TS$_{FG}$**	1.024962	−5235.997712	104.37i
^{1}**E**	1.035654	−5236.027174	^{5}**TS$_{FG}$**	1.022767	−5236.002718	109.90i
^{OSS}**E**	1.033322	−5236.031343	^{OSS}**TS$_{G2m'}$**	1.019298	−5234.827241	35.59i
^{3}**E**	1.032582	−5236.036783	^{3}**TS$_{G2m'}$**	1.017378	−5234.821643	16.97i
^{OSS}**F**	1.029836	−5236.012925	^{5}**TS$_{G2m'}$**	1.016017	−5234.824114	85.41i
^{3}**F**	1.028498	−5236.005829	^{1}**TS$_{2m'H}$**	1.022922	−5234.821244	67.61i
^{5}**F**	1.027028	−5236.011771	^{1}**TS$_{H2m}$**	1.017853	−5234.835468	220.18i
^{OSS}**G**	1.014795	−5234.829402	^{OSS}**TS$_{DE'}$**	1.022141	−5126.401438	729.03i
^{3}**G**	1.015720	−5234.824523	^{5}**TS$_{DE'}$**	1.018930	−5126.363819	354.94i
^{5}**G**	1.012730	−5234.826530	^{1}**TS$_{EF'}$**	1.034510	−5235.997248	375.89i
2m'	1.023738	−5234.851309	^{OSS}**TS$_{EF'}$**	1.032984	−5236.003923	215.79i
^{3}**2m'**	1.018471	−5234.844003	^{3}**TS$_{EF'}$**	1.029666	−5236.005320	210.28i
^{5}**2m'**	1.017082	−5234.821890	^{1}**TS$_{F'G'}$**	1.036882	−5235.999866	130.12i
^{1}**H**	1.018763	−5234.842610	^{3}**TS$_{F'G'}$**	1.034327	−5235.998947	97.10i
^{1}**2m**	1.022002	−5234.866693	^{1}**TS$_{F''G}$**	1.012483	−5234.776733	35.20i
^{3}**2m**	1.016410	−5234.856052	^{OSS}**TS$_{F''G}$**	1.006915	−5234.797518	27.75i
^{OSS}**E'**	1.022670	−5126.401906	^{3}**TS$_{F''G}$**	1.007543	−5234.788240	26.83i
^{5}**E'**	1.019750	−5126.397620	^{5}**TS$_{F''G}$**	1.006121	−5234.795906	26.90i
^{1}**F'**	1.036911	−5236.018686	^{1}**TS$_{HH'}$**	1.018554	−5234.832332	133.01i
^{3}**F'**	1.032079	−5236.012163	^{1}**TS$_{H'I}$**	1.016650	−5234.825997	15.95i
^{1}**F''**	1.009251	−5125.192571	^{1}**TS$_{IJ}$**	1.010790	−5234.820130	741.98i
^{OSS}**F''**	1.007643	−5125.213432	^{3}**TS$_{IJ}$**	1.010303	−5234.816582	409.24i
^{3}**F''**	1.009981	−5125.203065	^{1}**TS$_{JK}$**	1.011878	−5234.805533	185.80i
^{5}**F''**	1.005923	−5125.211358	^{OSS}**TS$_{JK}$**	1.010186	−5234.817176	193.58i
^{1}**H'**	1.017612	−5234.851124	^{3}**TS$_{JK}$**	1.007894	−5234.818311	221.57i
^{1}**I**	1.013758	−5234.827168	^{1}**TS$_{K5m}$**	0.998694	−5233.618895	547.58i
^{1}**J**	1.013623	−5234.821735	^{OSS}**TS$_{K5m}$**	0.999027	−5233.623411	529.12i
^{OSS}**J**	1.013251	−5234.825002	^{3}**TS$_{K5m}$**	0.997839	−5233.627738	455.14i
^{3}**J**	1.013352	−5234.830972	^{1}**TS$_{[2m-1]}$**	1.015829	−5234.793087	97.89i

^{1}**K**	1.000152	−5233.633639	^{OSS}**TS**$_{[2m-1]}$	1.014274	−5234.797957	129.63i
^{OSS}**K**	1.000132	−5233.643517	^{3}**TS**$_{[2m-1]}$	1.014526	−5234.803166	122.49i
^{3}**K**	0.999614	−5233.644044	^{1}**TS**$_{[2m-2]}$	1.020053	−5234.805635	775.97i
^{1}**5m**	1.006027	−5233.727709	^{OSS}**TS**$_{[2m-2]}$	1.017632	−5234.806412	541.33i
			^{3}**TS**$_{[2m-2]}$	1.016266	−5234.805796	731.66i
			^{1}**TS**$_{[2m-3]}$	1.018741	−5234.793025	1123.85i
			^{OSS}**TS**$_{[2m-3]}$	1.015470	−5234.792654	1078.62i
			^{3}**TS**$_{[2m-3]}$	1.014537	−5234.796622	1131.68i
			^{1}**TS**$_{[H'-1]}$	1.017694	−5234.804945	159.71i
			^{3}**TS**$_{[H'-1]}$	1.012595	−5234.812463	148.76i
			^{1}**TS**$_{[H'-2]}$	1.015083	−5234.798235	1074.40i
			^{OSS}**TS**$_{[H'-2]}$	1.016009	−5234.806213	1066.46i
			^{3}**TS**$_{[H'-2]}$	1.014960	−5234.805799	855.82i
			^{1}**TS**$_{[H'-3]}$	1.017691	−5234.805576	804.92i

(b) H_2 elimination of **2m**^{L1}, **2m**^{L2}, and **2m**^{L3} at TPSSTPSS/BSII//TPSSTPSS/BSI level

species	$\Delta\Delta G_{gas}$	E_{sp}	species	$\Delta\Delta G_{gas}$	E_{sp}	*IF*
^{1}**2m**^{L1}	1.006046	−5158.586536	^{1}**TS**$_{IJ}^{L1}$	0.996712	−5158.529377	911.44i
^{1}**2m**^{L2}	0.964940	−5156.222792	^{1}**TS**$_{H'I}^{L2}$	0.961574	−5156.189891	74.09i
^{1}**2m**^{L3}	0.128929	−3294.661268	^{1}**TS**$_{IJ}^{L2}$	0.957055	−5156.190007	603.56i
^{1}**2m'**^{L3}	0.129734	−3294.644937	^{1}**TS**$_{IJ}^{L3}$	0.124743	−3294.612343	870.79i
			^{1}**TS'**$_{IJ}^{L3}$	0.124641	−3294.616348	779.14i

Optimized Cartesian coordinates for all of the stationary points

H_2

H	0.000000000	0.000000000	0.370085000
H	0.000000000	0.000000000	-0.370085000

N_2

N	0.000000000	0.000000000	0.557124000
N	0.000000000	0.000000000	-0.557124000

1m(doublet)

Ti	0.038287000	-1.141726000	-0.579336000
P	-2.446067000	-0.876465000	0.043731000
P	2.544239000	-0.741422000	0.032676000
N	-0.021157000	0.936662000	-0.164266000
C	1.152652000	1.702515000	0.041223000
C	3.547489000	1.828783000	0.628619000
H	4.493821000	1.316582000	0.809768000
C	-3.764207000	3.041646000	-0.152669000
C	-1.251546000	1.644371000	-0.182229000
C	1.151896000	3.128683000	0.023329000
C	-1.321465000	3.063570000	-0.284247000
C	-2.550661000	3.731144000	-0.245348000
H	-2.548404000	4.820433000	-0.315126000
C	-0.056391000	3.851032000	-0.516962000
C	-2.501727000	0.946160000	-0.087711000
C	-3.722634000	1.647009000	-0.087490000
H	-4.655710000	1.086949000	-0.033085000
C	2.287872000	3.853446000	0.396643000
H	2.228740000	4.943399000	0.396961000
C	2.413390000	1.068460000	0.285359000
C	-4.230371000	-0.846844000	2.330114000
H	-4.384741000	0.236511000	2.237150000
H	-4.351887000	-1.111603000	3.391316000
H	-5.021533000	-1.361401000	1.768636000
C	3.492652000	3.220471000	0.727834000
C	-2.819386000	-1.245210000	1.862018000
H	-2.708214000	-2.337768000	1.942482000
C	0.037994000	-3.015680000	0.496900000
H	-0.796753000	-3.259697000	1.174789000
H	0.963626000	-3.349765000	0.991176000
H	-0.089339000	-3.659680000	-0.402764000
C	-1.738974000	-0.583632000	2.740042000
H	-0.732264000	-0.906561000	2.446326000
H	-1.894263000	-0.858380000	3.794008000
H	-1.785830000	0.510741000	2.660797000
C	-3.948333000	-1.521356000	-0.892239000
H	-4.846569000	-1.054679000	-0.459135000
C	3.935873000	-0.966526000	-1.242411000
H	4.886109000	-0.906069000	-0.685751000
C	3.345315000	-1.304846000	1.652597000
H	4.195275000	-0.618748000	1.799159000
C	3.893321000	-2.743944000	1.612886000
H	3.105318000	-3.472521000	1.382138000
H	4.307923000	-3.000774000	2.599201000
H	4.698840000	-2.859083000	0.876542000
C	0.030882000	-1.297477000	-2.696787000
H	-0.073463000	-2.349738000	-3.017985000
H	0.952596000	-0.896152000	-3.155742000
H	-0.810103000	-0.724122000	-3.127464000
C	-3.866468000	-1.141228000	-2.383377000
H	-3.792244000	-0.055200000	-2.521790000
H	-4.769040000	-1.493311000	-2.904618000
H	-2.995000000	-1.608912000	-2.859486000
C	-4.051667000	-3.050733000	-0.713480000
H	-3.146239000	-3.550402000	-1.084887000
H	-4.910020000	-3.434003000	-1.284456000
H	-4.193174000	-3.338640000	0.336805000
C	2.360471000	-1.108675000	2.821205000
H	1.983972000	-0.078251000	2.859329000
H	2.867195000	-1.322930000	3.774086000
H	1.505160000	-1.790029000	2.729533000
C	3.927213000	0.130160000	-2.325326000
H	2.970198000	0.146780000	-2.863893000
H	4.720595000	-0.078232000	-3.058781000
H	4.097620000	1.127092000	-1.903997000
C	3.814812000	-2.361784000	-1.894513000
H	3.810652000	-3.175232000	-1.158783000
H	4.660771000	-2.527111000	-2.578565000
H	2.885762000	-2.432362000	-2.475595000
H	-4.713393000	3.574817000	-0.142594000
H	0.078571000	4.005161000	-1.605644000
H	-0.139129000	4.857283000	-0.079375000
H	4.369779000	3.798162000	1.014585000

methane

C	0.000000000	0.000000000	0.000000000
H	0.632664000	0.632664000	0.632664000
H	-0.632664000	-0.632664000	0.632664000
H	-0.632664000	0.632664000	-0.632664000
H	0.632664000	-0.632664000	-0.632664000

TS_{1mA}(doublet)

Ti	0.066222000	-1.159294000	-0.556801000
P	-2.388662000	-0.782980000	0.117097000
P	2.504183000	-0.696314000	0.136575000
N	0.011059000	0.977390000	-0.260863000
C	1.185228000	1.745612000	-0.067863000
C	3.567210000	1.884930000	0.564943000
H	4.494544000	1.373064000	0.827119000
C	-3.673832000	3.147794000	0.052535000
C	-1.205754000	1.702922000	-0.196822000
C	1.202268000	3.166109000	-0.194279000
C	-1.263491000	3.117507000	-0.361336000
C	-2.468571000	3.810738000	-0.210610000
H	-2.459878000	4.895478000	-0.330522000
C	-0.010197000	3.841813000	-0.781025000
C	-2.445573000	1.034415000	0.044419000
C	-3.649912000	1.755081000	0.156086000
H	-4.580743000	1.212994000	0.321749000
C	2.343947000	3.902995000	0.134344000
H	2.302068000	4.989982000	0.045917000
C	2.423796000	1.120064000	0.266496000
C	-4.454460000	-1.277069000	2.124556000
H	-4.874108000	-0.267410000	2.019325000
H	-4.648001000	-1.605883000	3.156681000
H	-5.001157000	-1.952894000	1.455029000
C	3.533560000	3.280776000	0.536560000
C	-2.934674000	-1.281192000	1.868794000
H	-2.561545000	-2.312201000	1.973230000
C	0.085918000	-3.512418000	-0.144215000
H	-0.008536000	-4.127480000	0.765064000
H	1.037621000	-3.779620000	-0.626122000
H	-0.735428000	-3.793199000	-0.817473000
C	-2.216823000	-0.394742000	2.908130000
H	-1.132344000	-0.371067000	2.743965000
H	-2.405902000	-0.785251000	3.919022000
H	-2.591038000	0.636473000	2.861645000
C	-3.782373000	-1.352333000	-1.017961000
H	-4.723907000	-0.990229000	-0.576429000
C	3.905715000	-0.923145000	-1.119188000
H	4.789960000	-0.444074000	-0.666764000
C	3.262392000	-1.303104000	1.767845000
H	4.346337000	-1.116641000	1.683874000
C	3.028620000	-2.813823000	1.980651000
H	1.961316000	-3.020050000	2.127943000

H	3.565738000	-3.144367000	2.882217000
H	3.373230000	-3.425494000	1.139018000
C	0.093046000	-1.757168000	-2.608807000
H	0.991824000	-2.353403000	-2.850143000
H	0.088865000	-0.865419000	-3.263550000
H	-0.774430000	-2.383555000	-2.882896000
C	-3.635657000	-0.736211000	-2.423206000
H	-3.674801000	0.359137000	-2.388272000
H	-4.455592000	-1.090474000	-3.065814000
H	-2.686816000	-1.031803000	-2.888874000
C	-3.822843000	-2.892912000	-1.085531000
H	-2.910120000	-3.284568000	-1.552901000
H	-4.680750000	-3.216687000	-1.693020000
H	-3.919355000	-3.355199000	-0.093658000
C	2.714015000	-0.513130000	2.973212000
H	2.939875000	0.556828000	2.903618000
H	3.160218000	-0.904464000	3.899806000
H	1.623812000	-0.627710000	3.048161000
C	3.568099000	-0.188123000	-2.431626000
H	2.675733000	-0.616213000	-2.906052000
H	4.409000000	-0.289529000	-3.133966000
H	3.390036000	0.880409000	-2.261643000
C	4.229957000	-2.405890000	-1.388351000
H	4.617591000	-2.916707000	-0.498364000
H	4.999986000	-2.475583000	-2.171062000
H	3.342998000	-2.949194000	-1.741648000
H	-4.606408000	3.700615000	0.152568000
H	0.066718000	3.822961000	-1.886190000
H	-0.051373000	4.902518000	-0.494070000
H	4.414852000	3.868081000	0.788926000
H	0.080269000	-1.503818000	1.344614000
H	0.064852000	-2.303194000	0.914008000

A(doublet)

Ti	0.066222000	-1.159294000	-0.556801000
P	-2.388662000	-0.782980000	0.117097000
P	2.504183000	-0.696314000	0.136575000
N	0.011059000	0.977390000	-0.260863000
C	1.185228000	1.745612000	-0.067863000
C	3.567210000	1.884930000	0.564943000
H	4.494544000	1.373064000	0.827119000
C	-3.673832000	3.147794000	0.052535000
C	-1.205754000	1.702922000	-0.196822000
C	1.202268000	3.166109000	-0.194279000
C	-1.263491000	3.117507000	-0.361336000
C	-2.468571000	3.810738000	-0.210610000
H	-2.459878000	4.895478000	-0.330522000
C	-0.010197000	3.841813000	-0.781025000
C	-2.445573000	1.034415000	0.044419000
C	-3.649912000	1.755081000	0.156086000
H	-4.580743000	1.212994000	0.321749000
C	2.343947000	3.902995000	0.134344000
H	2.302068000	4.989982000	0.045917000
C	2.423796000	1.120064000	0.266496000
C	-4.454460000	-1.277069000	2.124556000
H	-4.874108000	-0.267410000	2.019325000
H	-4.648001000	-1.605883000	3.156681000
H	-5.001157000	-1.952894000	1.455029000
C	3.533560000	3.280776000	0.536560000
C	-2.934674000	-1.281192000	1.868794000
H	-2.561545000	-2.312201000	1.973230000
C	0.085918000	-3.512418000	-0.144215000
H	-0.008536000	-4.127480000	0.765064000
H	1.037621000	-3.779620000	-0.626122000
H	-0.735428000	-3.793199000	-0.817473000
C	-2.216823000	-0.394742000	2.908130000
H	-1.132344000	-0.371067000	2.743965000
H	-2.405902000	-0.785251000	3.919022000
H	-2.591038000	0.636473000	2.861645000
C	-3.782373000	-1.352333000	-1.017961000
H	-4.723907000	-0.990229000	-0.576429000
C	3.905715000	-0.923145000	-1.119188000
H	4.789960000	-0.444074000	-0.666764000
C	3.262392000	-1.303104000	1.767845000
H	4.346337000	-1.116641000	1.683874000
C	3.028620000	-2.813823000	1.980651000
H	1.961316000	-3.020050000	2.127943000
H	3.565738000	-3.144367000	2.882217000
H	3.373230000	-3.425494000	1.139018000
C	0.093046000	-1.757168000	-2.608807000
H	0.991824000	-2.353403000	-2.850143000
H	0.088865000	-0.865419000	-3.263550000
H	-0.774430000	-2.383555000	-2.882896000
C	-3.635657000	-0.736211000	-2.423206000
H	-3.674801000	0.359137000	-2.388272000
H	-4.455592000	-1.090474000	-3.065814000
H	-2.686816000	-1.031803000	-2.888874000
C	-3.822843000	-2.892912000	-1.085531000
H	-2.910120000	-3.284568000	-1.552901000
H	-4.680750000	-3.216687000	-1.693020000
H	-3.919355000	-3.355199000	-0.093658000
C	2.714015000	-0.513130000	2.973212000
H	2.939875000	0.556828000	2.903618000
H	3.160218000	-0.904464000	3.899806000
H	1.623812000	-0.627710000	3.048161000
C	3.568099000	-0.188123000	-2.431626000
H	2.675733000	-0.616213000	-2.906052000
H	4.409000000	-0.289529000	-3.133966000
H	3.390036000	0.880409000	-2.261643000
C	4.229957000	-2.405890000	-1.388351000
H	4.617591000	-2.916707000	-0.498364000
H	4.999986000	-2.475583000	-2.171062000
H	3.342998000	-2.949194000	-1.741648000
H	-4.606408000	3.700615000	0.152568000
H	0.066718000	3.822961000	-1.886190000
H	-0.051373000	4.902518000	-0.494070000
H	4.414852000	3.868081000	0.788926000
H	0.080269000	-1.503818000	1.344614000
H	0.064852000	-2.303194000	0.914008000

TS_{AB}(doublet)

Ti	0.071587000	-1.184774000	-0.717681000
P	-2.306584000	-0.920022000	0.138807000
P	2.444106000	-0.816029000	0.082728000
N	-0.009531000	0.890887000	-0.383592000
C	1.133799000	1.650008000	-0.043148000
C	3.430267000	1.755490000	0.826067000
H	4.336015000	1.240530000	1.150217000
C	-3.749509000	2.954224000	-0.346106000
C	-1.241475000	1.590898000	-0.373161000
C	1.134985000	3.072741000	-0.091025000
C	-1.311878000	3.002456000	-0.525280000
C	-2.547819000	3.658414000	-0.496378000
H	-2.565326000	4.743433000	-0.613245000
C	-0.027066000	3.758781000	-0.772666000
C	-2.468081000	0.879856000	-0.180286000
C	-3.696981000	1.564836000	-0.189276000
H	-4.622946000	1.004455000	-0.059108000
C	2.229201000	3.796493000	0.394197000
H	2.188765000	4.886869000	0.366719000
C	2.335807000	0.998342000	0.369455000
C	-4.059645000	-0.959159000	2.449307000
H	-4.454861000	0.032772000	2.188990000
H	-4.117663000	-1.059511000	3.543562000
H	-4.716995000	-1.722243000	2.012907000
C	3.376342000	3.152346000	0.878697000
C	-2.592422000	-1.102673000	2.003798000
H	-2.234476000	-2.120261000	2.221417000

C	-1.701849000	-0.098618000	2.761712000
H	-0.661423000	-0.158414000	2.422918000
H	-1.736571000	-0.317614000	3.839301000
H	-2.058880000	0.928885000	2.609415000
C	-3.816854000	-1.722233000	-0.654179000
H	-4.715047000	-1.282589000	-0.193794000
C	3.978716000	-0.875666000	-1.042683000
H	4.788882000	-0.403707000	-0.462671000
C	3.084319000	-1.614404000	1.676591000
H	4.177869000	-1.468879000	1.673128000
C	2.764457000	-3.124514000	1.682787000
H	1.677994000	-3.272986000	1.641846000
H	3.153857000	-3.578994000	2.606594000
H	3.206805000	-3.655897000	0.831497000
C	0.083226000	-1.960945000	-2.840807000
H	0.991001000	-1.371057000	-3.063359000
H	-0.805813000	-1.354835000	-3.094690000
H	0.088799000	-2.837119000	-3.500135000
C	-3.863484000	-1.447975000	-2.169590000
H	-3.859650000	-0.372970000	-2.390765000
H	-4.777998000	-1.883566000	-2.598819000
H	-3.006677000	-1.910663000	-2.678394000
C	-3.799286000	-3.239069000	-0.368553000
H	-2.888768000	-3.700198000	-0.775380000
H	-4.669875000	-3.719336000	-0.839360000
H	-3.834237000	-3.459431000	0.706671000
C	2.495110000	-0.947055000	2.933214000
H	2.728969000	0.122858000	2.985131000
H	2.903519000	-1.436715000	3.830197000
H	1.404196000	-1.064450000	2.946986000
C	3.760318000	-0.047017000	-2.322975000
H	2.981942000	-0.493306000	-2.958135000
H	4.689208000	-0.022227000	-2.912214000
H	3.470590000	0.986019000	-2.095658000
C	4.395971000	-2.318066000	-1.389117000
H	4.715501000	-2.880720000	-0.503452000
H	5.240956000	-2.300205000	-2.093977000
H	3.571405000	-2.867876000	-1.865015000
H	-4.704293000	3.477827000	-0.345732000
H	0.170085000	3.795551000	-1.862467000
H	-0.117658000	4.804102000	-0.443201000
H	4.219305000	3.728082000	1.257748000
H	0.164027000	-1.667478000	0.948765000
H	0.075274000	-3.034547000	-0.609155000
H	0.076149000	-2.728961000	-1.697746000

B(doublet)

Ti	0.062184000	-1.174760000	-0.721558000
P	-2.371053000	-1.004999000	-0.021511000
P	2.501120000	-0.896835000	-0.050207000
N	0.004920000	0.827411000	-0.269290000
C	1.181742000	1.575637000	0.004336000
C	3.555358000	1.643252000	0.653522000
H	4.484566000	1.111054000	0.862751000
C	-3.728219000	2.917428000	-0.082443000
C	-1.227705000	1.535427000	-0.217125000
C	1.186857000	2.997231000	0.026708000
C	-1.290094000	2.953933000	-0.271184000
C	-2.520242000	3.616707000	-0.181988000
H	-2.525503000	4.707469000	-0.216929000
C	-0.019319000	3.736888000	-0.500601000
C	-2.465170000	0.824418000	-0.098959000
C	-3.687296000	1.520163000	-0.054275000
H	-4.618471000	0.957661000	0.008013000
C	2.327354000	3.697027000	0.438381000
H	2.285443000	4.787157000	0.468362000
C	2.417355000	0.910109000	0.272893000
C	-4.305112000	-1.239879000	2.121674000
H	-4.550489000	-0.169937000	2.085820000
H	-4.480308000	-1.585506000	3.151478000
H	-5.002676000	-1.779887000	1.467540000
C	3.514540000	3.035572000	0.775847000
C	-2.831984000	-1.481420000	1.745654000
H	-2.615808000	-2.560193000	1.782885000
C	-1.882046000	-0.765879000	2.726259000
H	-0.834127000	-0.968153000	2.472369000
H	-2.069408000	-1.122325000	3.749939000
H	-2.044589000	0.320338000	2.706893000
C	-3.755462000	-1.639930000	-1.122654000
H	-4.710009000	-1.233614000	-0.753355000
C	3.841060000	-0.955814000	-1.385541000
H	4.717769000	-0.429873000	-0.973297000
C	3.258543000	-1.683933000	1.490399000
H	4.338028000	-1.459926000	1.464283000
C	3.046469000	-3.213118000	1.483364000
H	1.972099000	-3.439423000	1.486443000
H	3.501318000	-3.649360000	2.385391000
H	3.495110000	-3.702089000	0.610673000
C	-3.527812000	-1.154994000	-2.569370000
H	-3.547516000	-0.059722000	-2.634547000
H	-4.319055000	-1.552498000	-3.222297000
H	-2.557532000	-1.504114000	-2.950555000
C	-3.804348000	-3.180602000	-1.051920000
H	-2.853019000	-3.615250000	-1.388892000
H	-4.601529000	-3.557153000	-1.709348000
H	-4.006548000	-3.545613000	-0.035815000
C	2.645365000	-1.076552000	2.768017000
H	2.824767000	0.002348000	2.841495000
H	3.084989000	-1.563878000	3.650990000
H	1.561157000	-1.250929000	2.789477000
C	3.336334000	-0.192508000	-2.628290000
H	2.437080000	-0.671649000	-3.041553000
H	4.115784000	-0.196012000	-3.404861000
H	3.095139000	0.851452000	-2.391692000
C	4.247128000	-2.394545000	-1.757965000
H	4.741558000	-2.915566000	-0.928709000
H	4.954210000	-2.366310000	-2.600383000
H	3.374553000	-2.983938000	-2.072026000
H	-4.677595000	3.448277000	-0.034342000
H	0.111598000	3.902445000	-1.587835000
H	-0.092882000	4.737453000	-0.049392000
H	4.392478000	3.594018000	1.096465000
H	0.107919000	-2.246315000	0.696656000
H	0.078241000	-1.617794000	-2.455460000

C(closed-shell singlet)

Ti	1.347624000	0.489644000	-0.445657000
P	1.274062000	-1.187023000	-2.383277000
P	2.776447000	2.375803000	0.477633000
N	3.049381000	-0.636158000	-0.070401000
C	4.073355000	-0.118554000	0.771208000
C	5.207260000	1.793916000	1.819245000
H	5.246972000	2.865095000	2.019549000
C	3.703270000	-4.505388000	-1.761891000
C	3.262567000	-1.937244000	-0.599279000
C	5.068719000	-0.958062000	1.344050000
C	4.214517000	-2.835697000	-0.050934000
C	4.436494000	-4.083942000	-0.647391000
H	5.186008000	-4.744278000	-0.207724000
C	4.919901000	-2.456338000	1.227934000
C	2.508948000	-2.374616000	-1.730301000
C	2.728992000	-3.646995000	-2.284709000
H	2.132843000	-3.968330000	-3.138340000
C	6.132985000	-0.408390000	2.068617000
H	6.891951000	-1.082460000	2.469463000
C	4.139084000	1.278599000	1.062440000
C	1.991532000	-1.509247000	-5.194692000
H	2.529463000	-2.442682000	-4.976778000

H	2.485767000	-1.040444000	-6.059272000
H	0.966557000	-1.759272000	-5.496908000
C	6.225133000	0.967854000	2.304958000
C	2.045305000	-0.543498000	-3.996488000
H	1.451870000	0.356021000	-4.219823000
C	3.497086000	-0.107765000	-3.723343000
H	3.549203000	0.544568000	-2.844205000
H	3.891105000	0.440967000	-4.591828000
H	4.140262000	-0.980589000	-3.547045000
C	-0.169780000	-2.242861000	-2.971090000
H	0.215476000	-2.912639000	-3.755531000
C	2.392820000	3.363763000	2.055838000
H	3.318212000	3.902853000	2.318728000
C	3.644481000	3.677690000	-0.605540000
H	4.070200000	4.406649000	0.104605000
C	2.649532000	4.398838000	-1.536769000
H	2.171376000	3.673375000	-2.207460000
H	3.188660000	5.142150000	-2.144041000
H	1.860193000	4.924295000	-0.987023000
C	-0.739307000	-3.096972000	-1.826983000
H	0.003416000	-3.804453000	-1.438447000
H	-1.606942000	-3.670608000	-2.186571000
H	-1.073273000	-2.457806000	-0.998837000
C	-1.256035000	-1.333512000	-3.580647000
H	-1.649900000	-0.645607000	-2.821980000
H	-2.089782000	-1.947134000	-3.953203000
H	-0.877938000	-0.733975000	-4.420052000
C	4.791344000	3.073593000	-1.437425000
H	5.555744000	2.600050000	-0.810915000
H	5.269477000	3.870714000	-2.026797000
H	4.405876000	2.323427000	-2.138528000
C	2.007968000	2.425963000	3.214829000
H	1.089646000	1.876989000	2.968708000
H	1.821003000	3.023604000	4.120327000
H	2.803112000	1.704289000	3.439841000
C	1.268321000	4.387387000	1.813118000
H	1.549019000	5.156333000	1.082285000
H	1.026817000	4.898959000	2.757185000
H	0.361459000	3.876483000	1.462688000
H	3.878844000	-5.483768000	-2.206476000
H	4.331219000	-2.827427000	2.089599000
H	5.899844000	-2.951593000	1.295619000
H	7.058521000	1.382939000	2.869695000
H	1.611785000	1.498953000	-1.849368000
H	0.380140000	0.834102000	1.039617000
Ti	-1.333709000	0.484111000	0.423288000
P	-1.274704000	-1.189296000	2.379017000
P	-2.775224000	2.377973000	-0.465356000
N	-3.047233000	-0.631390000	0.063158000
C	-4.024516000	-0.129326000	-0.840978000
C	-5.071212000	1.759551000	-2.015888000
H	-5.091881000	2.824587000	-2.247159000
C	-3.867124000	-4.405045000	1.888469000
C	-3.305744000	-1.906843000	0.630593000
C	-4.999084000	-0.975333000	-1.439418000
C	-4.265471000	-2.800928000	0.087586000
C	-4.550504000	-4.011232000	0.732768000
H	-5.306866000	-4.666859000	0.297776000
C	-4.897607000	-2.468722000	-1.241628000
C	-2.587343000	-2.325999000	1.790301000
C	-2.869155000	-3.563679000	2.393679000
H	-2.299092000	-3.874095000	3.268775000
C	-6.004810000	-0.440597000	-2.252900000
H	-6.748092000	-1.119533000	-2.674373000
C	-4.064061000	1.261409000	-1.168787000
C	-1.872066000	-1.454385000	5.225300000
H	-2.494224000	-2.343047000	5.049704000
H	-2.274647000	-0.943228000	6.113043000
H	-0.853793000	-1.783550000	5.468355000
C	-6.058736000	0.926031000	-2.548302000
C	-1.921835000	-0.492535000	4.023465000
H	-1.258426000	0.365352000	4.212134000
C	-3.351697000	0.042344000	3.821663000
H	-3.389432000	0.725823000	2.965727000
H	-3.675736000	0.587989000	4.720580000
H	-4.057190000	-0.781083000	3.645540000
C	0.135541000	-2.324813000	2.901027000
H	-0.252978000	-2.974065000	3.700992000
C	-2.363366000	3.488985000	-1.948609000
H	-3.304525000	3.986516000	-2.236029000
C	-3.744571000	3.582339000	0.649743000
H	-4.098395000	4.375745000	-0.030123000
C	-2.839577000	4.212323000	1.727447000
H	-2.440592000	3.433459000	2.389295000
H	-3.425187000	4.926133000	2.327100000
H	-1.987407000	4.752284000	1.297691000
C	0.600634000	-3.207777000	1.731569000
H	-0.199109000	-3.872232000	1.382052000
H	1.451991000	-3.828773000	2.048536000
H	0.928673000	-2.588802000	0.886241000
C	1.299962000	-1.484386000	3.461486000
H	1.705572000	-0.825907000	2.683297000
H	2.107205000	-2.149331000	3.803558000
H	0.995818000	-0.859944000	4.312634000
C	-4.972316000	2.920630000	1.304615000
H	-5.693637000	2.561916000	0.561736000
H	-5.476555000	3.653907000	1.952257000
H	-4.675263000	2.069383000	1.929655000
C	-1.843363000	2.665005000	-3.140409000
H	-0.908697000	2.154342000	-2.874152000
H	-1.642343000	3.337671000	-3.988517000
H	-2.574505000	1.914339000	-3.466397000
C	-1.338472000	4.568148000	-1.553636000
H	-1.728166000	5.257447000	-0.793458000
H	-1.071402000	5.164941000	-2.438742000
H	-0.422130000	4.100587000	-1.170730000
H	-4.092145000	-5.354110000	2.372522000
H	-4.277931000	-2.899550000	-2.052243000
H	-5.886795000	-2.941156000	-1.333964000
H	-6.844341000	1.329263000	-3.185480000
H	-1.552206000	1.477452000	1.837157000
H	-0.367654000	0.882631000	-1.046662000

C(open-shell singlet)

Ti	-1.399189000	-0.446920000	-0.550677000
P	-1.450436000	1.318075000	-2.398090000
P	-2.699792000	-2.407853000	0.426446000
N	-3.114188000	0.584131000	-0.008765000
C	-4.078921000	0.011896000	0.864426000
C	-5.100743000	-1.975108000	1.886422000
H	-5.097864000	-3.053790000	2.046760000
C	-3.883879000	4.544089000	-1.435141000
C	-3.364971000	1.909718000	-0.453894000
C	-5.067490000	0.797170000	1.518094000
C	-4.303093000	2.762940000	0.186868000
C	-4.563748000	4.042473000	-0.320091000
H	-5.301941000	4.662879000	0.191173000
C	-4.958893000	2.302333000	1.466252000
C	-2.670263000	2.427905000	-1.592695000
C	-2.927190000	3.731439000	-2.052823000
H	-2.373440000	4.113034000	-2.910253000
C	-6.078645000	0.186134000	2.269509000
H	-6.835129000	0.819415000	2.736325000
C	-4.084722000	-1.395297000	1.106186000
C	-2.310559000	1.846833000	-5.128708000
H	-2.878613000	2.732064000	-4.810277000
H	-2.816873000	1.432359000	-6.013644000
H	-1.309089000	2.168767000	-5.442032000

C	-6.119747000	-1.200981000	2.450661000
C	-2.276409000	0.780092000	-4.018711000
H	-1.663712000	-0.073483000	-4.346323000
C	-3.696806000	0.266507000	-3.716864000
H	-3.680584000	-0.471742000	-2.906911000
H	-4.119486000	-0.207389000	-4.615299000
H	-4.356572000	1.093299000	-3.420870000
C	-0.035254000	2.433928000	-2.940669000
H	-0.445232000	3.175639000	-3.643578000
C	-2.207153000	-3.426031000	1.953494000
H	-3.106449000	-3.995606000	2.241598000
C	-3.573369000	-3.701882000	-0.660856000
H	-3.980288000	-4.447981000	0.042611000
C	-2.595120000	-4.395689000	-1.629409000
H	-2.138752000	-3.651372000	-2.294792000
H	-3.143653000	-5.128276000	-2.241300000
H	-1.790320000	-4.929164000	-1.110955000
C	0.572622000	3.172944000	-1.736081000
H	-0.161492000	3.824167000	-1.245875000
H	1.416388000	3.795792000	-2.069584000
H	0.950719000	2.456669000	-0.993358000
C	1.029963000	1.588101000	-3.668457000
H	1.444340000	0.828773000	-2.993144000
H	1.853966000	2.235132000	-4.004112000
H	0.624786000	1.075041000	-4.551516000
C	-4.739163000	-3.087292000	-1.458565000
H	-5.493631000	-2.630134000	-0.808254000
H	-5.224875000	-3.874030000	-2.055669000
H	-4.367547000	-2.321417000	-2.150520000
C	-1.796133000	-2.506882000	3.118021000
H	-0.900210000	-1.932689000	2.847064000
H	-1.558946000	-3.122115000	3.999836000
H	-2.598206000	-1.810769000	3.393139000
C	-1.068547000	-4.414867000	1.640971000
H	-1.356908000	-5.170885000	0.900121000
H	-0.783588000	-4.945039000	2.562444000
H	-0.184255000	-3.874600000	1.277635000
H	-4.088217000	5.546255000	-1.808721000
H	-4.354120000	2.648170000	2.327424000
H	-5.947877000	2.769303000	1.586033000
H	-6.912951000	-1.664145000	3.035585000
H	-1.723803000	-1.458671000	-1.954583000
H	-0.399185000	-0.445048000	1.000307000
Ti	1.357484000	-0.549785000	0.454498000
P	1.408949000	1.015797000	2.503710000
P	2.847513000	-2.301070000	-0.676852000
N	3.040652000	0.654518000	0.074162000
C	3.963556000	0.265450000	-0.938989000
C	4.995144000	-1.486485000	-2.329420000
H	5.038289000	-2.531126000	-2.637998000
C	3.960416000	4.279571000	2.154506000
C	3.326321000	1.885728000	0.728072000
C	4.860749000	1.191349000	-1.542385000
C	4.219083000	2.849612000	0.187879000
C	4.542573000	4.003914000	0.912554000
H	5.245798000	4.712685000	0.471751000
C	4.728175000	2.658131000	-1.218109000
C	2.700384000	2.194938000	1.972020000
C	3.017530000	3.378208000	2.660884000
H	2.513325000	3.601227000	3.600511000
C	5.818902000	0.762479000	-2.468420000
H	6.499303000	1.503945000	-2.890663000
C	4.039061000	-1.092988000	-1.374988000
C	2.123964000	1.117260000	5.327666000
H	2.832306000	1.942965000	5.175060000
H	2.482535000	0.532141000	6.188168000
H	1.148355000	1.539971000	5.600245000
C	5.903605000	-0.574250000	-2.872140000
C	2.056758000	0.205487000	4.088378000
H	1.334860000	-0.605861000	4.268282000
C	3.429752000	-0.432691000	3.806938000
H	3.364365000	-1.119189000	2.954457000
H	3.765492000	-1.000661000	4.687643000
H	4.183530000	0.335756000	3.586141000
C	-0.000978000	2.117968000	3.091125000
H	0.412914000	2.761985000	3.882984000
C	2.360935000	-3.328935000	-2.192118000
H	3.294694000	-3.784574000	-2.561821000
C	3.920127000	-3.535265000	0.303199000
H	4.262590000	-4.277482000	-0.437648000
C	3.097481000	-4.253662000	1.392371000
H	2.706662000	-3.527701000	2.116219000
H	3.738101000	-4.976868000	1.920045000
H	2.240926000	-4.800603000	0.979860000
C	-0.508144000	3.012840000	1.946934000
H	0.286310000	3.659897000	1.555041000
H	-1.326422000	3.652922000	2.309958000
H	-0.897381000	2.402026000	1.121821000
C	-1.146032000	1.273125000	3.682385000
H	-1.578411000	0.621708000	2.913617000
H	-1.939332000	1.938020000	4.056001000
H	-0.814575000	0.643771000	4.519402000
C	5.158792000	-2.859667000	0.924060000
H	5.828322000	-2.447738000	0.160531000
H	5.719096000	-3.600437000	1.514441000
H	4.869728000	-2.042729000	1.597643000
C	1.754256000	-2.454461000	-3.304639000
H	0.818858000	-1.992053000	-2.964668000
H	1.532675000	-3.085171000	-4.179408000
H	2.444381000	-1.662391000	-3.621179000
C	1.387664000	-4.457923000	-1.803439000
H	1.834549000	-5.173683000	-1.101665000
H	1.093573000	-5.015500000	-2.705270000
H	0.478560000	-4.040630000	-1.352624000
H	4.213758000	5.186985000	2.700433000
H	4.016226000	3.125034000	-1.926409000
H	5.686480000	3.178006000	-1.364071000
H	6.652009000	-0.894262000	-3.595412000
H	1.422184000	-1.647993000	1.815932000
H	0.366657000	-0.919314000	-1.017449000

C(triplet)

Ti	1.327858000	0.458489000	-0.582814000
P	1.549275000	-1.262291000	-2.482062000
P	2.635163000	2.335015000	0.562394000
N	3.007531000	-0.634945000	0.047746000
C	3.825902000	-0.149393000	1.105061000
C	4.665570000	1.734940000	2.447837000
H	4.638383000	2.798174000	2.687902000
C	4.190463000	-4.365992000	-1.689065000
C	3.374639000	-1.896496000	-0.494543000
C	4.709970000	-0.992233000	1.834323000
C	4.257941000	-2.786601000	0.176714000
C	4.673002000	-3.975766000	-0.434978000
H	5.367726000	-4.621187000	0.105452000
C	4.659401000	-2.480748000	1.598114000
C	2.849960000	-2.322754000	-1.753962000
C	3.254453000	-3.543146000	-2.323632000
H	2.823451000	-3.856777000	-3.273558000
C	5.570958000	-0.460468000	2.801692000
H	6.245278000	-1.139784000	3.326062000
C	3.804568000	1.234316000	1.454918000
C	2.375102000	-1.684375000	-5.243590000
H	3.153260000	-2.412815000	-4.979412000
H	2.691655000	-1.188344000	-6.173582000
H	1.446150000	-2.228030000	-5.458977000
C	5.566076000	0.902435000	3.118625000
C	2.208086000	-0.624965000	-4.137812000

H	1.441489000	0.102574000	-4.446824000
C	3.525530000	0.139501000	-3.910732000
H	3.379578000	0.943736000	-3.180271000
H	3.865906000	0.584367000	-4.857898000
H	4.313765000	-0.533875000	-3.546184000
C	0.186447000	-2.476730000	-2.947903000
H	0.638737000	-3.226959000	-3.615512000
C	1.997248000	3.482197000	1.932072000
H	2.870877000	4.075339000	2.251174000
C	3.803560000	3.476174000	-0.419253000
H	4.187978000	4.205008000	0.314332000
C	3.075172000	4.230277000	-1.549349000
H	2.631913000	3.516800000	-2.255803000
H	3.795125000	4.864057000	-2.089564000
H	2.273500000	4.879558000	-1.177844000
C	-0.342870000	-3.192844000	-1.691554000
H	0.454600000	-3.732641000	-1.165479000
H	-1.117376000	-3.920286000	-1.978773000
H	-0.795052000	-2.471914000	-0.997020000
C	-0.952998000	-1.756411000	-3.695020000
H	-1.410415000	-0.992059000	-3.055104000
H	-1.731873000	-2.483347000	-3.969823000
H	-0.607807000	-1.271877000	-4.618528000
C	4.996021000	2.685594000	-0.994955000
H	5.618652000	2.249710000	-0.205644000
H	5.622276000	3.359173000	-1.599361000
H	4.650991000	1.871907000	-1.645628000
C	1.450715000	2.696689000	3.138532000
H	0.577214000	2.103725000	2.838066000
H	1.132908000	3.410045000	3.914840000
H	2.204259000	2.029499000	3.573314000
C	0.911054000	4.439998000	1.405368000
H	1.270680000	5.089088000	0.597814000
H	0.568794000	5.087580000	2.226739000
H	0.047606000	3.866331000	1.044822000
H	4.512839000	-5.300319000	-2.145840000
H	3.918737000	-2.933355000	2.286215000
H	5.624769000	-2.948339000	1.842089000
H	6.240077000	1.303101000	3.874257000
H	1.551823000	1.543054000	-1.951966000
H	0.448147000	0.515838000	1.036346000
Ti	-1.325786000	0.545810000	0.500523000
P	-1.549541000	-0.847234000	2.651311000
P	-2.635523000	2.214274000	-0.928535000
N	-3.005785000	-0.634952000	0.053028000
C	-3.823666000	-0.325780000	-1.068833000
C	-4.662390000	1.318620000	-2.697125000
H	-4.635467000	2.329646000	-3.104623000
C	-4.192536000	-4.036646000	2.367455000
C	-3.373822000	-1.792633000	0.791139000
C	-4.706850000	-1.274945000	-1.654232000
C	-4.256913000	-2.779003000	0.271123000
C	-4.673153000	-3.853851000	1.066085000
H	-5.367625000	-4.577727000	0.635983000
C	-4.656883000	-2.706049000	-1.181438000
C	-2.850633000	-2.010512000	2.103384000
C	-3.256924000	-3.122505000	2.862290000
H	-2.827567000	-3.278844000	3.851091000
C	-5.566563000	-0.905682000	-2.695576000
H	-6.240128000	-1.660591000	-3.104928000
C	-3.802795000	0.984164000	-1.635422000
C	-2.374410000	-0.819221000	5.444629000
H	-3.149547000	-1.583712000	5.300575000
H	-2.694561000	-0.180558000	6.281735000
H	-1.444107000	-1.317555000	5.746530000
C	-5.561463000	0.388688000	-3.227124000
C	-2.208553000	0.048289000	4.182470000
H	-1.442810000	0.817069000	4.369381000
C	-3.527109000	0.763930000	3.835124000
H	-3.382662000	1.438300000	2.983183000
H	-3.867014000	1.357019000	4.697459000
H	-4.314852000	0.039336000	3.586042000
C	-0.188641000	-1.972178000	3.308080000
H	-0.642709000	-2.604305000	4.087337000
C	-1.999584000	3.129671000	-2.463702000
H	-2.876062000	3.656940000	-2.876751000
C	-3.804516000	3.495907000	-0.139790000
H	-4.186395000	4.101841000	-0.978931000
C	-3.076957000	4.416115000	0.860244000
H	-2.636198000	3.821348000	1.670540000
H	-3.796766000	5.127645000	1.293190000
H	-2.273245000	4.997912000	0.393541000
C	0.341453000	-2.882647000	2.185080000
H	-0.455546000	-3.500394000	1.752349000
H	1.115096000	-3.554219000	2.587588000
H	0.794911000	-2.283746000	1.383753000
C	0.950831000	-1.142689000	3.931473000
H	1.410792000	-0.492724000	3.177315000
H	1.727700000	-1.816914000	4.322036000
H	0.604706000	-0.514507000	4.763572000
C	-4.999235000	2.806563000	0.549906000
H	-5.622021000	2.254959000	-0.163177000
H	-5.624501000	3.566956000	1.041885000
H	-4.656549000	2.102782000	1.319116000
C	-1.443720000	2.163273000	-3.525966000
H	-0.567681000	1.632095000	-3.131723000
H	-1.127614000	2.744072000	-4.406489000
H	-2.191796000	1.429851000	-3.849311000
C	-0.922477000	4.168659000	-2.096902000
H	-1.290753000	4.939126000	-1.408812000
H	-0.580097000	4.674830000	-3.012201000
H	-0.057305000	3.668784000	-1.643034000
H	-4.516212000	-4.884786000	2.968638000
H	-3.915661000	-3.263645000	-1.786887000
H	-5.622193000	-3.206619000	-1.347933000
H	-6.234347000	0.662544000	-4.038307000
H	-1.552407000	1.833547000	1.679825000
H	-0.446597000	0.349322000	-1.107691000

TS_{CD}(closed-shell singlet)

Ti	1.457395000	0.408302000	-0.526063000
P	1.428282000	-1.413070000	-2.246896000
P	2.921731000	2.378897000	0.289533000
N	3.143270000	-0.646074000	0.063542000
C	4.161607000	-0.074541000	0.870292000
C	5.348061000	1.914579000	1.694276000
H	5.423327000	3.000465000	1.761791000
C	3.671222000	-4.728077000	-1.091330000
C	3.311332000	-2.015406000	-0.285645000
C	5.109436000	-0.870781000	1.571794000
C	4.198635000	-2.875736000	0.412472000
C	4.381521000	-4.199429000	-0.008420000
H	5.082374000	-4.828818000	0.542802000
C	4.887689000	-2.361957000	1.653382000
C	2.580833000	-2.560019000	-1.385227000
C	2.762255000	-3.901835000	-1.762300000
H	2.187297000	-4.305281000	-2.595334000
C	6.182566000	-0.271802000	2.241780000
H	6.905434000	-0.915281000	2.746270000
C	4.272808000	1.343352000	0.990772000
C	2.267325000	-2.132848000	-4.951790000
H	2.748196000	-3.051068000	-4.585778000
H	2.827078000	-1.801925000	-5.839929000
H	1.248566000	-2.378839000	-5.277711000
C	6.327748000	1.119630000	2.297558000
C	2.304832000	-1.021458000	-3.886728000
H	1.763352000	-0.137575000	-4.256758000
C	3.760417000	-0.609095000	-3.596846000

H	3.803038000	0.146142000	-2.803780000
H	4.217709000	-0.190193000	-4.505808000
H	4.355522000	-1.476502000	-3.280629000
C	-0.013540000	-2.514466000	-2.772079000
H	0.394378000	-3.284329000	-3.445285000
C	2.531582000	3.499854000	1.771204000
H	3.469613000	4.027756000	2.010567000
C	3.785948000	3.569670000	-0.913602000
H	4.215261000	4.365227000	-0.281348000
C	2.783550000	4.192053000	-1.906582000
H	2.302820000	3.401408000	-2.497465000
H	3.317581000	4.869652000	-2.590262000
H	1.997225000	4.770475000	-1.408175000
C	-0.661004000	-3.210132000	-1.563574000
H	0.046815000	-3.863853000	-1.039918000
H	-1.514642000	-3.819590000	-1.896897000
H	-1.038147000	-2.469809000	-0.845000000
C	-1.046636000	-1.673325000	-3.546675000
H	-1.458266000	-0.887280000	-2.898715000
H	-1.878193000	-2.311739000	-3.880559000
H	-0.613745000	-1.189097000	-4.432916000
C	4.927194000	2.883212000	-1.687487000
H	5.690027000	2.465151000	-1.020790000
H	5.408748000	3.618779000	-2.349476000
H	4.533983000	2.073601000	-2.314450000
C	2.101224000	2.658075000	2.986765000
H	1.181142000	2.103528000	2.756665000
H	1.899883000	3.324126000	3.839993000
H	2.879571000	1.945356000	3.286325000
C	1.447153000	4.538415000	1.431811000
H	1.763282000	5.235024000	0.645149000
H	1.216318000	5.133029000	2.328753000
H	0.526664000	4.034285000	1.111137000
H	3.815333000	-5.762390000	-1.400152000
H	4.257172000	-2.583435000	2.536627000
H	5.838282000	-2.890066000	1.819457000
H	7.169746000	1.572272000	2.818961000
H	1.798955000	1.183977000	-2.065720000
H	0.270165000	-0.655040000	0.399440000
Ti	-1.249454000	0.315453000	0.192718000
P	-1.557281000	-0.884738000	2.394538000
P	-2.791975000	2.297142000	-0.606218000
N	-3.102637000	-0.627339000	-0.061741000
C	-4.059793000	-0.153796000	-0.989945000
C	-5.059218000	1.705843000	-2.243820000
H	-5.064801000	2.762798000	-2.512138000
C	-4.248036000	-4.072247000	2.164138000
C	-3.472140000	-1.798618000	0.650503000
C	-5.033216000	-1.016379000	-1.566558000
C	-4.433704000	-2.709638000	0.144048000
C	-4.822807000	-3.814175000	0.912845000
H	-5.572758000	-4.495776000	0.507840000
C	-4.945838000	-2.494216000	-1.261862000
C	-2.868114000	-2.073642000	1.910483000
C	-3.258270000	-3.206157000	2.646040000
H	-2.780311000	-3.415571000	3.602888000
C	-6.007244000	-0.501533000	-2.427977000
H	-6.749953000	-1.183934000	-2.844646000
C	-4.088036000	1.227125000	-1.344014000
C	-2.379769000	-0.669911000	5.196543000
H	-3.019915000	-1.558526000	5.104151000
H	-2.836325000	-0.013798000	5.953594000
H	-1.400653000	-0.983747000	5.580196000
C	-6.030573000	0.855607000	-2.780196000
C	-2.279932000	0.085488000	3.858728000
H	-1.583828000	0.931450000	3.967272000
C	-3.655671000	0.636988000	3.444520000
H	-3.599608000	1.115748000	2.459012000
H	-4.007970000	1.378139000	4.177336000
H	-4.397759000	-0.171099000	3.386121000
C	-0.226988000	-1.954269000	3.197990000
H	-0.692886000	-2.428091000	4.076361000
C	-2.217219000	3.301463000	-2.104683000
H	-3.109089000	3.841284000	-2.465553000
C	-3.694367000	3.652926000	0.394612000
H	-3.799373000	4.498513000	-0.304917000
C	-2.822208000	4.105195000	1.583832000
H	-2.643376000	3.274766000	2.277967000
H	-3.329087000	4.915579000	2.129783000
H	-1.842566000	4.475157000	1.258292000
C	0.272106000	-3.064500000	2.255248000
H	-0.544124000	-3.724278000	1.935014000
H	1.022876000	-3.677255000	2.777492000
H	0.742879000	-2.635198000	1.362994000
C	0.941842000	-1.067138000	3.669932000
H	1.410859000	-0.569643000	2.811429000
H	1.703344000	-1.686800000	4.167475000
H	0.621111000	-0.292752000	4.380378000
C	-5.103722000	3.241006000	0.860061000
H	-5.764299000	3.010983000	0.016427000
H	-5.549829000	4.068147000	1.432995000
H	-5.074611000	2.359703000	1.512238000
C	-1.693610000	2.390448000	-3.230576000
H	-0.807582000	1.833682000	-2.896260000
H	-1.403719000	3.008055000	-4.094672000
H	-2.457944000	1.677075000	-3.564267000
C	-1.147065000	4.329056000	-1.695787000
H	-1.518131000	5.049317000	-0.954077000
H	-0.824157000	4.898428000	-2.580259000
H	-0.271202000	3.813753000	-1.282878000
H	-4.552045000	-4.942810000	2.743560000
H	-4.247617000	-2.971591000	-1.976754000
H	-5.919472000	-2.983733000	-1.408363000
H	-6.788938000	1.238837000	-3.461187000
H	-0.438690000	1.294408000	1.426769000
H	-0.131824000	1.341302000	-0.783632000

TS_{CD}(open-shell singlet)

Ti	1.504616000	0.449631000	-0.518761000
P	1.474435000	-1.308193000	-2.348260000
P	2.964973000	2.336617000	0.447762000
N	3.164723000	-0.672628000	0.038684000
C	4.156507000	-0.162540000	0.917471000
C	5.320388000	1.758017000	1.924412000
H	5.397379000	2.836551000	2.067953000
C	3.739737000	-4.663844000	-1.386898000
C	3.342906000	-2.013106000	-0.400342000
C	5.076454000	-1.009609000	1.597139000
C	4.212434000	-2.921836000	0.260104000
C	4.415658000	-4.210677000	-0.248981000
H	5.102904000	-4.875543000	0.277251000
C	4.851784000	-2.501823000	1.561267000
C	2.640730000	-2.485369000	-1.551739000
C	2.841256000	-3.796555000	-2.018149000
H	2.286178000	-4.144223000	-2.888962000
C	6.123365000	-0.465811000	2.350234000
H	6.823444000	-1.148072000	2.835658000
C	4.273617000	1.244303000	1.138063000
C	2.302617000	-1.883706000	-5.087455000
H	2.825980000	-2.797434000	-4.772857000
H	2.828789000	-1.492640000	-5.971582000
H	1.286419000	-2.154290000	-5.402049000
C	6.270371000	0.917177000	2.512036000
C	2.322599000	-0.819515000	-3.974810000
H	1.753589000	0.064645000	-4.300308000
C	3.768659000	-0.378165000	-3.679179000
H	3.791912000	0.363977000	-2.872843000
H	4.212939000	0.069398000	-4.580898000

H	4.385676000	-1.236499000	-3.380677000
C	0.029983000	-2.392924000	-2.897309000
H	0.432485000	-3.133385000	-3.605671000
C	2.486819000	3.353380000	1.974160000
H	3.410610000	3.850564000	2.313765000
C	3.881762000	3.594695000	-0.639869000
H	4.287869000	4.348770000	0.055327000
C	2.921522000	4.280165000	-1.633488000
H	2.471468000	3.529707000	-2.296358000
H	3.481877000	5.004151000	-2.244708000
H	2.109511000	4.820581000	-1.133161000
C	-0.599271000	-3.141877000	-1.709512000
H	0.123644000	-3.801019000	-1.213712000
H	-1.440165000	-3.757205000	-2.064270000
H	-0.987844000	-2.435494000	-0.964029000
C	-1.019989000	-1.530595000	-3.624724000
H	-1.443956000	-0.783926000	-2.940338000
H	-1.842955000	-2.165554000	-3.985247000
H	-0.600403000	-0.997913000	-4.489171000
C	5.051042000	2.945459000	-1.404715000
H	5.788937000	2.495154000	-0.730966000
H	5.556103000	3.710994000	-2.012962000
H	4.682954000	2.165979000	-2.083597000
C	1.970443000	2.425382000	3.089521000
H	1.051883000	1.916019000	2.764431000
H	1.731610000	3.024365000	3.981942000
H	2.717487000	1.673528000	3.373369000
C	1.431198000	4.425907000	1.646199000
H	1.798892000	5.173636000	0.932093000
H	1.154215000	4.957223000	2.569381000
H	0.525357000	3.956968000	1.240858000
H	3.898317000	-5.672726000	-1.764879000
H	4.185742000	-2.785601000	2.399757000
H	5.794794000	-3.043576000	1.726667000
H	7.091298000	1.326462000	3.098787000
H	1.848101000	1.334394000	-2.008511000
H	0.216146000	-0.542968000	0.380940000
Ti	-1.335056000	0.437344000	0.362091000
P	-1.641434000	-0.934425000	2.487459000
P	-2.781011000	2.320271000	-0.691708000
N	-3.142733000	-0.590109000	-0.010749000
C	-4.020918000	-0.158539000	-1.037800000
C	-4.916758000	1.648231000	-2.449428000
H	-4.897359000	2.693794000	-2.758243000
C	-4.392429000	-4.047690000	2.162385000
C	-3.538459000	-1.769043000	0.677674000
C	-4.954088000	-1.037839000	-1.656568000
C	-4.473645000	-2.688251000	0.132203000
C	-4.905192000	-3.786929000	0.885698000
H	-5.638163000	-4.465089000	0.445144000
C	-4.907389000	-2.504514000	-1.302267000
C	-2.982942000	-2.063158000	1.957765000
C	-3.411035000	-3.192594000	2.676990000
H	-2.963370000	-3.411698000	3.646013000
C	-5.858256000	-0.558350000	-2.610307000
H	-6.569172000	-1.259026000	-3.051529000
C	-4.015898000	1.204893000	-1.463350000
C	-2.518949000	-0.826774000	5.264370000
H	-3.274639000	-1.607669000	5.102667000
H	-2.889240000	-0.171819000	6.067767000
H	-1.597319000	-1.301632000	5.625128000
C	-5.852303000	0.781239000	-3.020438000
C	-2.298543000	0.007637000	3.989884000
H	-1.518399000	0.761568000	4.174198000
C	-3.587252000	0.744035000	3.583611000
H	-3.411964000	1.347933000	2.685339000
H	-3.915830000	1.409475000	4.396065000
H	-4.397214000	0.032052000	3.372294000
C	-0.332533000	-2.087238000	3.205876000
H	-0.810606000	-2.624839000	4.039933000
C	-2.128860000	3.298570000	-2.171851000
H	-3.007674000	3.794955000	-2.616455000
C	-3.779449000	3.649186000	0.239704000
H	-3.971321000	4.441346000	-0.503358000
C	-2.949131000	4.241919000	1.397350000
H	-2.696198000	3.467458000	2.131395000
H	-3.528092000	5.031814000	1.899893000
H	-2.005689000	4.680690000	1.051022000
C	0.143675000	-3.121223000	2.168540000
H	-0.685959000	-3.735176000	1.795886000
H	0.883387000	-3.791298000	2.632670000
H	0.621125000	-2.624046000	1.315451000
C	0.854125000	-1.270123000	3.752589000
H	1.341180000	-0.715423000	2.940725000
H	1.597248000	-1.948148000	4.198778000
H	0.548938000	-0.550874000	4.524898000
C	-5.136307000	3.122811000	0.746379000
H	-5.784217000	2.801936000	-0.077300000
H	-5.650626000	3.921951000	1.301334000
H	-5.008442000	2.270772000	1.425820000
C	-1.494665000	2.366720000	-3.220549000
H	-0.620515000	1.849260000	-2.800187000
H	-1.155067000	2.963967000	-4.080757000
H	-2.211354000	1.620648000	-3.586343000
C	-1.123991000	4.379409000	-1.731441000
H	-1.574199000	5.122170000	-1.059975000
H	-0.752251000	4.914907000	-2.617849000
H	-0.265668000	3.917477000	-1.228528000
H	-4.728348000	-4.914180000	2.729957000
H	-4.182789000	-3.016583000	-1.965210000
H	-5.880547000	-2.982947000	-1.485586000
H	-6.558241000	1.137815000	-3.768887000
H	-1.044024000	1.518359000	1.713863000
H	-0.063639000	1.483245000	-0.446790000

TS_{CD}(triplet)

Ti	1.384314000	0.452103000	-0.540928000
P	1.562453000	-1.276885000	-2.391104000
P	2.747364000	2.415079000	0.430043000
N	3.118395000	-0.568003000	0.052521000
C	4.119854000	0.017503000	0.872963000
C	5.226678000	2.022076000	1.768990000
H	5.254945000	3.107015000	1.878160000
C	3.910149000	-4.539270000	-1.331675000
C	3.382129000	-1.896714000	-0.382253000
C	5.106448000	-0.762987000	1.538523000
C	4.302204000	-2.749128000	0.285103000
C	4.563965000	-4.036109000	-0.201629000
H	5.283041000	-4.658561000	0.333862000
C	4.943987000	-2.263560000	1.561612000
C	2.725606000	-2.411554000	-1.541476000
C	2.985611000	-3.719306000	-1.987823000
H	2.462963000	-4.097351000	-2.866253000
C	6.157285000	-0.145695000	2.227069000
H	6.908800000	-0.777190000	2.704269000
C	4.170652000	1.432351000	1.052109000
C	2.485782000	-1.800227000	-5.118265000
H	2.968870000	-2.736724000	-4.805109000
H	3.065096000	-1.400703000	-5.964674000
H	1.479611000	-2.034091000	-5.489590000
C	6.244388000	1.247552000	2.335206000
C	2.478419000	-0.767455000	-3.976166000
H	1.936489000	0.134510000	-4.299671000
C	3.919960000	-0.358542000	-3.615120000
H	3.932180000	0.327600000	-2.760407000
H	4.390995000	0.142074000	-4.474334000
H	4.521431000	-1.241227000	-3.358979000
C	0.167931000	-2.387335000	-3.014274000

H	0.619176000	-3.078613000	-3.742721000
C	2.308343000	3.424711000	1.975816000
H	3.222488000	3.982575000	2.238874000
C	3.509709000	3.737088000	-0.702675000
H	3.898883000	4.517791000	-0.027158000
C	2.449039000	4.351977000	-1.637730000
H	2.026177000	3.569666000	-2.281660000
H	2.918955000	5.118211000	-2.273358000
H	1.625870000	4.827133000	-1.091627000
C	-0.482387000	-3.220559000	-1.895131000
H	0.245956000	-3.869840000	-1.394059000
H	-1.269435000	-3.857640000	-2.327755000
H	-0.941760000	-2.572519000	-1.138939000
C	-0.886525000	-1.527180000	-3.739916000
H	-1.366070000	-0.835515000	-3.034823000
H	-1.668023000	-2.172926000	-4.167662000
H	-0.454849000	-0.932518000	-4.556916000
C	4.674656000	3.177386000	-1.540049000
H	5.478819000	2.770941000	-0.915782000
H	5.091865000	3.981544000	-2.165231000
H	4.315195000	2.382633000	-2.205243000
C	1.934067000	2.497585000	3.146277000
H	1.025690000	1.931422000	2.900305000
H	1.731682000	3.103088000	4.043430000
H	2.741321000	1.793738000	3.384119000
C	1.171042000	4.428354000	1.706104000
H	1.455168000	5.195315000	0.974619000
H	0.911139000	4.945217000	2.642725000
H	0.276300000	3.903299000	1.347219000
H	4.114942000	-5.546432000	-1.691720000
H	4.304589000	-2.543425000	2.421650000
H	5.910987000	-2.760917000	1.727298000
H	7.070120000	1.715261000	2.869280000
H	1.956467000	1.324064000	-1.955504000
H	0.015361000	-0.750188000	-0.138519000
Ti	-1.352198000	0.421923000	0.247039000
P	-1.342884000	-0.977556000	2.397676000
P	-2.991645000	2.213998000	-0.707555000
N	-3.159454000	-0.691017000	0.086410000
C	-4.163118000	-0.314066000	-0.844417000
C	-5.295574000	1.424416000	-2.174147000
H	-5.355734000	2.463772000	-2.498900000
C	-3.979770000	-4.195949000	2.384094000
C	-3.410172000	-1.886962000	0.807238000
C	-5.116689000	-1.244437000	-1.349023000
C	-4.356811000	-2.855014000	0.375965000
C	-4.647003000	-3.967756000	1.174489000
H	-5.391386000	-4.683031000	0.820244000
C	-4.956081000	-2.704148000	-1.000655000
C	-2.697591000	-2.148747000	2.014989000
C	-2.986249000	-3.293350000	2.779229000
H	-2.421009000	-3.485484000	3.690630000
C	-6.145479000	-0.822164000	-2.197914000
H	-6.865884000	-1.563321000	-2.548376000
C	-4.265808000	1.037390000	-1.297318000
C	-2.042191000	-0.873026000	5.225260000
H	-2.828724000	-1.630259000	5.104393000
H	-2.338986000	-0.217035000	6.057789000
H	-1.112930000	-1.378384000	5.519491000
C	-6.252848000	0.509041000	-2.620047000
C	-1.880634000	-0.032868000	3.946084000
H	-1.073594000	0.701653000	4.090153000
C	-3.173272000	0.737565000	3.623288000
H	-3.028860000	1.371952000	2.739624000
H	-3.454947000	1.381416000	4.470038000
H	-4.004801000	0.047349000	3.423763000
C	0.049763000	-2.091071000	3.007426000
H	-0.357024000	-2.640472000	3.871106000
C	-2.546295000	3.174932000	-2.272330000
H	-3.487927000	3.620816000	-2.633546000
C	-3.933893000	3.523428000	0.306494000
H	-4.270001000	4.270624000	-0.431863000
C	-2.999791000	4.213557000	1.322258000
H	-2.616822000	3.492090000	2.054131000
H	-3.554994000	4.997029000	1.860215000
H	-2.132631000	4.681339000	0.841846000
C	0.470439000	-3.112824000	1.935279000
H	-0.371237000	-3.745623000	1.627152000
H	1.259563000	-3.764210000	2.340157000
H	0.866607000	-2.606412000	1.047517000
C	1.251267000	-1.251463000	3.480452000
H	1.681271000	-0.685604000	2.644331000
H	2.032873000	-1.917323000	3.876070000
H	0.981776000	-0.542664000	4.274888000
C	-5.178177000	2.944006000	1.007687000
H	-5.905962000	2.550258000	0.289225000
H	-5.664326000	3.737093000	1.595632000
H	-4.910504000	2.132144000	1.695633000
C	-1.987978000	2.238231000	-3.359382000
H	-1.046753000	1.781849000	-3.025779000
H	-1.783543000	2.818885000	-4.271761000
H	-2.698469000	1.441832000	-3.614802000
C	-1.547875000	4.307589000	-1.967100000
H	-1.970935000	5.067293000	-1.297166000
H	-1.268245000	4.811003000	-2.904588000
H	-0.635607000	3.901545000	-1.513080000
H	-4.208032000	-5.071921000	2.989262000
H	-4.283635000	-3.182449000	-1.739713000
H	-5.917449000	-3.233151000	-1.074223000
H	-7.055389000	0.820332000	-3.286780000
H	-0.724345000	1.561317000	1.441759000
H	-0.254267000	1.350419000	-0.866370000

D(closed-shell singlet)

Ti	1.276377000	0.460598000	-0.389477000
P	1.286482000	-1.130425000	-2.383220000
P	2.885866000	2.290829000	0.448725000
N	3.047538000	-0.655768000	-0.044404000
C	4.084597000	-0.184319000	0.807992000
C	5.258116000	1.683151000	1.908509000
H	5.325301000	2.751393000	2.119193000
C	3.682366000	-4.484618000	-1.826171000
C	3.259375000	-1.942250000	-0.600490000
C	5.034872000	-1.061435000	1.404811000
C	4.174987000	-2.879693000	-0.051754000
C	4.387412000	-4.115764000	-0.674520000
H	5.100454000	-4.810124000	-0.226635000
C	4.836397000	-2.551199000	1.263515000
C	2.540224000	-2.324291000	-1.772505000
C	2.747474000	-3.588319000	-2.355381000
H	2.174579000	-3.874160000	-3.236787000
C	6.086399000	-0.555162000	2.177163000
H	6.802543000	-1.259854000	2.603664000
C	4.203563000	1.206900000	1.109318000
C	2.201308000	-1.481804000	-5.148768000
H	2.894438000	-2.280684000	-4.852776000
H	2.630420000	-0.977653000	-6.028314000
H	1.253686000	-1.938833000	-5.462142000
C	6.220186000	0.815466000	2.433488000
C	2.017065000	-0.462279000	-4.010862000
H	1.291114000	0.302133000	-4.333489000
C	3.352099000	0.239333000	-3.695502000
H	3.235255000	0.997259000	-2.908865000
H	3.744172000	0.740967000	-4.592756000
H	4.101757000	-0.485023000	-3.349398000
C	-0.134592000	-2.218920000	-2.969081000
H	0.294271000	-2.861044000	-3.754296000
C	2.449841000	3.405143000	1.914659000

H	3.380792000	3.941415000	2.165517000
C	3.757959000	3.537088000	-0.709380000
H	3.983741000	4.408872000	-0.073668000
C	2.804761000	3.991202000	-1.834682000
H	2.567605000	3.157794000	-2.510876000
H	3.281363000	4.781524000	-2.434416000
H	1.857233000	4.381792000	-1.446020000
C	-0.680022000	-3.125445000	-1.851299000
H	0.107639000	-3.754424000	-1.418922000
H	-1.455412000	-3.785977000	-2.268766000
H	-1.124666000	-2.529527000	-1.047302000
C	-1.251877000	-1.362675000	-3.594862000
H	-1.699039000	-0.703738000	-2.840730000
H	-2.044209000	-2.016905000	-3.988228000
H	-0.888408000	-0.741365000	-4.425325000
C	5.083307000	3.009620000	-1.291306000
H	5.815634000	2.787892000	-0.507195000
H	5.512871000	3.768120000	-1.963414000
H	4.932104000	2.091617000	-1.873919000
C	1.994390000	2.589088000	3.137140000
H	1.057680000	2.062700000	2.914338000
H	1.816217000	3.271531000	3.982382000
H	2.751723000	1.856670000	3.443677000
C	1.369104000	4.429489000	1.520022000
H	1.692024000	5.087857000	0.702042000
H	1.136419000	5.067192000	2.386127000
H	0.450964000	3.908481000	1.219130000
H	3.849963000	-5.453014000	-2.295239000
H	4.192135000	-2.907939000	2.090688000
H	5.791702000	-3.086290000	1.368425000
H	7.039607000	1.191883000	3.043857000
H	-0.136397000	1.644995000	-0.556069000
H	0.457771000	0.642458000	1.210590000
Ti	-1.231979000	0.505041000	0.431446000
P	-1.360410000	-0.964437000	2.503104000
P	-2.862477000	2.273927000	-0.572344000
N	-2.986151000	-0.640183000	0.020606000
C	-3.971946000	-0.237695000	-0.917696000
C	-5.111744000	1.550778000	-2.171905000
H	-5.191302000	2.607443000	-2.431075000
C	-3.806486000	-4.296641000	2.076556000
C	-3.238497000	-1.876097000	0.669956000
C	-4.879622000	-1.160243000	-1.512444000
C	-4.127992000	-2.848565000	0.135588000
C	-4.417136000	-4.018304000	0.848012000
H	-5.114751000	-4.734956000	0.410938000
C	-4.680810000	-2.632371000	-1.251570000
C	-2.599448000	-2.175844000	1.911305000
C	-2.882785000	-3.378152000	2.585499000
H	-2.371622000	-3.598338000	3.521990000
C	-5.891751000	-0.713007000	-2.368607000
H	-6.576563000	-1.450313000	-2.791459000
C	-4.099100000	1.133942000	-1.290081000
C	-2.216796000	-1.098841000	5.297904000
H	-2.889771000	-1.943773000	5.096903000
H	-2.645658000	-0.529275000	6.136717000
H	-1.248792000	-1.495450000	5.630682000
C	-6.026518000	0.639606000	-2.708111000
C	-2.095214000	-0.181490000	4.067391000
H	-1.393016000	0.637107000	4.290643000
C	-3.456715000	0.443606000	3.715718000
H	-3.354981000	1.109440000	2.850544000
H	-3.836920000	1.028058000	4.567256000
H	-4.195316000	-0.333592000	3.474447000
C	0.037531000	-2.040445000	3.176289000
H	-0.407858000	-2.655363000	3.974202000
C	-2.372382000	3.330013000	-2.064680000
H	-3.307089000	3.783516000	-2.434826000
C	-3.867072000	3.529992000	0.452156000
H	-4.157765000	4.310477000	-0.271412000
C	-3.010379000	4.175384000	1.560244000
H	-2.691320000	3.421072000	2.289036000
H	-3.601992000	4.946815000	2.076971000
H	-2.102696000	4.648370000	1.166398000
C	0.609346000	-2.980662000	2.100564000
H	-0.163110000	-3.643187000	1.690315000
H	1.397515000	-3.607471000	2.546134000
H	1.044013000	-2.406552000	1.273600000
C	1.147458000	-1.166716000	3.793200000
H	1.613642000	-0.539284000	3.023880000
H	1.926584000	-1.810855000	4.228339000
H	0.771766000	-0.510537000	4.590544000
C	-5.153593000	2.921619000	1.044108000
H	-5.836721000	2.565856000	0.264675000
H	-5.674190000	3.687559000	1.638826000
H	-4.928677000	2.077285000	1.707059000
C	-1.769199000	2.462617000	-3.183943000
H	-0.866325000	1.949102000	-2.825498000
H	-1.492955000	3.099387000	-4.038729000
H	-2.481377000	1.706317000	-3.536020000
C	-1.405781000	4.459983000	-1.664167000
H	-1.863140000	5.170434000	-0.963710000
H	-1.105500000	5.023690000	-2.560601000
H	-0.503439000	4.042479000	-1.199627000
H	-4.031270000	-5.216110000	2.615095000
H	-3.967182000	-3.040092000	-1.993854000
H	-5.619807000	-3.187429000	-1.392770000
H	-6.815628000	0.970248000	-3.381710000
H	-1.310667000	1.689119000	1.712154000
H	0.014374000	-0.834632000	-0.058870000

D(open-shell singlet)

Ti	1.327969000	0.276396000	-0.066223000
P	1.499718000	-0.850156000	-2.391635000
P	2.929904000	2.221633000	0.662813000
N	3.132618000	-0.707905000	0.054744000
C	4.129876000	-0.282212000	0.967400000
C	5.208890000	1.512033000	2.242625000
H	5.254318000	2.560514000	2.538194000
C	4.084683000	-4.124636000	-2.287466000
C	3.438766000	-1.868937000	-0.699003000
C	5.085001000	-1.191236000	1.496343000
C	4.382659000	-2.822824000	-0.242915000
C	4.708629000	-3.920085000	-1.049783000
H	5.445736000	-4.638164000	-0.686963000
C	4.943067000	-2.657239000	1.152239000
C	2.787915000	-2.083408000	-1.945819000
C	3.112046000	-3.213543000	-2.717471000
H	2.597585000	-3.385407000	-3.662331000
C	6.092615000	-0.729275000	2.349937000
H	6.823479000	-1.443395000	2.732580000
C	4.204608000	1.088333000	1.351993000
C	2.172375000	-0.682890000	-5.240250000
H	2.772899000	-1.601667000	-5.190744000
H	2.608775000	-0.047417000	-6.025954000
H	1.155335000	-0.946635000	-5.556084000
C	6.163293000	0.616693000	2.735722000
C	2.201179000	0.074410000	-3.899618000
H	1.557460000	0.964532000	-3.980522000
C	3.634406000	0.534157000	-3.572708000
H	3.682943000	1.013173000	-2.587073000
H	3.986132000	1.252350000	-4.327935000
H	4.322591000	-0.321754000	-3.563209000
C	0.110165000	-1.900678000	-3.111455000
H	0.533975000	-2.400751000	-3.996705000
C	2.462542000	3.278633000	2.163320000
H	3.384374000	3.813093000	2.449125000
C	3.869066000	3.520560000	-0.383390000

H	4.024596000	4.375196000	0.295050000
C	2.990938000	3.987305000	-1.562414000
H	2.787966000	3.158797000	-2.253257000
H	3.507393000	4.782339000	-2.121430000
H	2.023848000	4.381734000	-1.227172000
C	-0.368834000	-2.981943000	-2.124948000
H	0.444909000	-3.660601000	-1.839835000
H	-1.162436000	-3.579017000	-2.598941000
H	-0.777259000	-2.528041000	-1.214844000
C	-1.058969000	-1.002448000	-3.559017000
H	-1.508321000	-0.500941000	-2.693282000
H	-1.834752000	-1.617449000	-4.039263000
H	-0.747648000	-0.233490000	-4.279701000
C	5.247748000	3.037737000	-0.871201000
H	5.922703000	2.814253000	-0.037260000
H	5.709541000	3.822892000	-1.488907000
H	5.166456000	2.132428000	-1.485801000
C	1.988579000	2.429191000	3.356116000
H	1.069943000	1.886181000	3.100492000
H	1.771996000	3.090503000	4.208837000
H	2.751112000	1.705513000	3.671048000
C	1.389874000	4.312941000	1.773473000
H	1.730047000	4.991780000	0.979672000
H	1.133428000	4.927575000	2.649110000
H	0.478807000	3.802762000	1.436431000
H	4.339198000	-4.989599000	-2.898035000
H	4.251950000	-3.133021000	1.874443000
H	5.905258000	-3.178879000	1.255916000
H	6.946967000	0.958702000	3.409893000
H	-0.214183000	1.033249000	-0.840389000
H	0.305796000	1.032228000	1.236508000
Ti	-1.400908000	0.438939000	0.539909000
P	-1.636267000	-1.350098000	2.331237000
P	-2.808078000	2.404247000	-0.324153000
N	-3.102629000	-0.590359000	-0.134619000
C	-4.104420000	0.008741000	-0.940145000
C	-5.256442000	2.026840000	-1.739274000
H	-5.320577000	3.115088000	-1.782118000
C	-3.796915000	-4.651125000	1.009964000
C	-3.335630000	-1.945436000	0.221364000
C	-5.046747000	-0.762610000	-1.677418000
C	-4.203562000	-2.790622000	-0.521414000
C	-4.431796000	-4.111091000	-0.114348000
H	-5.108968000	-4.729116000	-0.706796000
C	-4.824126000	-2.252094000	-1.787715000
C	-2.705074000	-2.495797000	1.378564000
C	-2.930354000	-3.834196000	1.745209000
H	-2.430285000	-4.238570000	2.625232000
C	-6.101178000	-0.138863000	-2.354080000
H	-6.818722000	-0.763290000	-2.889600000
C	-4.197331000	1.428718000	-1.034142000
C	-2.707436000	-2.009446000	4.978100000
H	-3.117511000	-2.957271000	4.600859000
H	-3.365581000	-1.669710000	5.792573000
H	-1.719667000	-2.206708000	5.414723000
C	-6.233611000	1.255342000	-2.377542000
C	-2.672248000	-0.938596000	3.872053000
H	-2.194191000	-0.025247000	4.258628000
C	-4.105769000	-0.580746000	3.432643000
H	-4.096386000	0.122843000	2.592317000
H	-4.648806000	-0.120088000	4.271670000
H	-4.652346000	-1.481767000	3.122714000
C	-0.246544000	-2.427843000	3.018313000
H	-0.717971000	-3.155963000	3.696348000
C	-2.373051000	3.501045000	-1.815250000
H	-3.299118000	4.038703000	-2.077542000
C	-3.634885000	3.663818000	0.837971000
H	-4.024723000	4.463550000	0.185266000
C	-2.615433000	4.262013000	1.828059000
H	-2.181931000	3.459082000	2.439236000
H	-3.122688000	4.978056000	2.493057000
H	-1.796172000	4.791753000	1.327702000
C	0.513669000	-3.209339000	1.932048000
H	-0.155752000	-3.847486000	1.342421000
H	1.271360000	-3.851376000	2.408343000
H	1.026691000	-2.527670000	1.242592000
C	0.719362000	-1.547507000	3.838859000
H	1.194676000	-0.796575000	3.193335000
H	1.511331000	-2.169052000	4.283507000
H	0.210341000	-1.015260000	4.654389000
C	-4.807399000	3.045326000	1.621538000
H	-5.582502000	2.639960000	0.960786000
H	-5.263692000	3.815384000	2.262490000
H	-4.444126000	2.237036000	2.267963000
C	-1.939368000	2.647835000	-3.020263000
H	-1.023346000	2.091649000	-2.782544000
H	-1.735674000	3.301451000	-3.882886000
H	-2.716621000	1.930321000	-3.310676000
C	-1.283624000	4.534865000	-1.474456000
H	-1.616451000	5.261083000	-0.722520000
H	-1.010364000	5.097218000	-2.380694000
H	-0.380797000	4.033250000	-1.100960000
H	-3.975670000	-5.683250000	1.308242000
H	-4.146481000	-2.452194000	-2.641087000
H	-5.764407000	-2.775078000	-2.016746000
H	-7.062421000	1.727993000	-2.902667000
H	-2.120327000	1.244069000	1.942218000
H	-0.104671000	-0.869516000	0.150586000

D(triplet)

Ti	1.302942000	0.283903000	-0.096524000
P	1.523731000	-0.916579000	-2.394043000
P	2.837628000	2.259816000	0.611338000
N	3.145835000	-0.656393000	0.064269000
C	4.139937000	-0.177692000	0.953075000
C	5.176514000	1.684567000	2.166061000
H	5.191367000	2.742107000	2.431850000
C	4.139972000	-4.154941000	-2.140586000
C	3.468182000	-1.839958000	-0.641698000
C	5.124869000	-1.041689000	1.502781000
C	4.435313000	-2.758951000	-0.158416000
C	4.772337000	-3.884397000	-0.919725000
H	5.526530000	-4.572272000	-0.533776000
C	5.013701000	-2.523220000	1.218948000
C	2.816603000	-2.117822000	-1.877933000
C	3.151831000	-3.276796000	-2.601494000
H	2.635660000	-3.494847000	-3.535955000
C	6.126389000	-0.525258000	2.332654000
H	6.878604000	-1.207333000	2.732498000
C	4.175447000	1.203982000	1.302139000
C	2.262946000	-0.864947000	-5.232715000
H	2.872652000	-1.772731000	-5.125910000
H	2.712618000	-0.259602000	-6.034651000
H	1.257849000	-1.155810000	-5.563340000
C	6.163352000	0.833418000	2.675237000
C	2.246662000	-0.048904000	-3.926976000
H	1.591329000	0.826047000	-4.063406000
C	3.663751000	0.450051000	-3.587168000
H	3.679840000	0.975434000	-2.624479000
H	4.022904000	1.137696000	-4.367023000
H	4.364721000	-0.392790000	-3.520275000
C	0.156750000	-2.005983000	-3.102902000
H	0.594817000	-2.527032000	-3.968597000
C	2.355577000	3.344253000	2.088171000
H	3.258752000	3.924506000	2.342295000
C	3.704349000	3.571998000	-0.484301000
H	3.817903000	4.457311000	0.162468000
C	2.798915000	3.950473000	-1.673567000

H	2.626069000	3.084896000	-2.326489000
H	3.274560000	4.743634000	-2.270599000
H	1.818124000	4.314786000	-1.344470000
C	-0.329565000	-3.064418000	-2.095203000
H	0.485388000	-3.726170000	-1.776144000
H	-1.107833000	-3.683417000	-2.567249000
H	-0.758739000	-2.589326000	-1.205490000
C	-1.013680000	-1.129975000	-3.589989000
H	-1.475078000	-0.606364000	-2.743416000
H	-1.781406000	-1.762559000	-4.060558000
H	-0.699220000	-0.379630000	-4.328884000
C	5.104908000	3.147828000	-0.964382000
H	5.795114000	2.989416000	-0.128065000
H	5.521165000	3.934624000	-1.611959000
H	5.069860000	2.218454000	-1.546619000
C	1.934254000	2.514688000	3.313645000
H	1.031356000	1.932860000	3.089754000
H	1.709517000	3.191571000	4.152190000
H	2.727757000	1.827295000	3.633322000
C	1.234364000	4.320933000	1.685437000
H	1.532537000	4.986061000	0.863488000
H	0.967057000	4.953712000	2.545044000
H	0.339861000	3.762709000	1.380577000
H	4.403151000	-5.041663000	-2.715318000
H	4.346782000	-2.985898000	1.972284000
H	5.989684000	-3.018136000	1.326788000
H	6.942730000	1.218302000	3.331178000
H	-0.246364000	1.168843000	-0.784663000
H	0.245353000	0.881442000	1.300372000
Ti	-1.412557000	0.456609000	0.495110000
P	-1.544275000	-1.248370000	2.370111000
P	-2.905195000	2.346201000	-0.423032000
N	-3.097394000	-0.641790000	-0.085639000
C	-4.113571000	-0.115468000	-0.927149000
C	-5.317152000	1.821618000	-1.846175000
H	-5.411110000	2.903429000	-1.949950000
C	-3.720992000	-4.632661000	1.315904000
C	-3.299759000	-1.979652000	0.352016000
C	-5.030739000	-0.953210000	-1.621480000
C	-4.155745000	-2.882728000	-0.332900000
C	-4.367116000	-4.175879000	0.161790000
H	-5.037757000	-4.839987000	-0.386291000
C	-4.776256000	-2.440908000	-1.635530000
C	-2.645033000	-2.449054000	1.529531000
C	-2.852829000	-3.762695000	1.985055000
H	-2.333545000	-4.106807000	2.879280000
C	-6.096166000	-0.398197000	-2.339879000
H	-6.793290000	-1.072435000	-2.840547000
C	-4.249205000	1.293593000	-1.099832000
C	-2.467038000	-1.778851000	5.100878000
H	-2.902858000	-2.741256000	4.796746000
H	-3.073763000	-1.394688000	5.935226000
H	-1.455665000	-1.960912000	5.486700000
C	-6.265794000	0.987737000	-2.447252000
C	-2.494165000	-0.763553000	3.943286000
H	-1.996849000	0.166659000	4.258703000
C	-3.949325000	-0.425968000	3.564307000
H	-3.983792000	0.240507000	2.694830000
H	-4.450127000	0.071253000	4.408593000
H	-4.509292000	-1.339287000	3.321540000
C	-0.112375000	-2.287859000	3.026746000
H	-0.550648000	-2.987769000	3.755079000
C	-2.480820000	3.398673000	-1.944376000
H	-3.421616000	3.889530000	-2.243652000
C	-3.773009000	3.616815000	0.694759000
H	-4.173866000	4.385142000	0.011864000
C	-2.780246000	4.272945000	1.675517000
H	-2.339271000	3.504975000	2.324479000
H	-3.312521000	5.004565000	2.302661000
H	-1.963296000	4.798068000	1.166779000
C	0.590519000	-3.112939000	1.934403000
H	-0.107823000	-3.774285000	1.407282000
H	1.373491000	-3.734658000	2.395931000
H	1.065996000	-2.459993000	1.192259000
C	0.893617000	-1.380446000	3.763970000
H	1.343544000	-0.661710000	3.066614000
H	1.701093000	-1.989697000	4.197175000
H	0.425950000	-0.810572000	4.578771000
C	-4.941933000	2.994597000	1.480903000
H	-5.697855000	2.551234000	0.822435000
H	-5.424801000	3.773405000	2.090672000
H	-4.573358000	2.215560000	2.159323000
C	-1.992060000	2.515114000	-3.105839000
H	-1.061726000	2.002619000	-2.829116000
H	-1.794449000	3.142666000	-3.988712000
H	-2.737682000	1.759909000	-3.383576000
C	-1.439308000	4.486195000	-1.621331000
H	-1.817806000	5.228624000	-0.907779000
H	-1.167369000	5.021361000	-2.543953000
H	-0.527515000	4.035212000	-1.208477000
H	-3.886936000	-5.644358000	1.683279000
H	-4.085961000	-2.680605000	-2.468016000
H	-5.703360000	-2.997024000	-1.837730000
H	-7.102075000	1.405712000	-3.005600000
H	-2.023257000	1.318660000	1.898603000
H	-0.180765000	-0.865965000	0.066397000

TS_{DE}(closed-shell singlet)

Ti	-1.247965000	0.416086000	0.152033000
P	-1.616479000	-0.496544000	2.518414000
P	-3.084558000	1.989588000	-1.001815000
N	-2.771593000	-0.925228000	-0.150795000
C	-3.762146000	-0.744383000	-1.146034000
C	-5.067831000	0.732801000	-2.603309000
H	-5.275032000	1.731888000	-2.988692000
C	-3.107795000	-4.381879000	2.294730000
C	-2.905519000	-2.086649000	0.649081000
C	-4.504601000	-1.844666000	-1.657314000
C	-3.590175000	-3.238451000	0.192880000
C	-3.693567000	-4.363039000	1.022904000
H	-4.222086000	-5.243005000	0.652817000
C	-4.126708000	-3.241876000	-1.219698000
C	-2.349290000	-2.085294000	1.958595000
C	-2.435981000	-3.241794000	2.754314000
H	-1.989851000	-3.247772000	3.748105000
C	-5.526912000	-1.631508000	-2.587769000
H	-6.091790000	-2.491615000	-2.950864000
C	-4.055584000	0.561079000	-1.638552000
C	-2.954509000	-0.520400000	5.152278000
H	-3.126122000	-1.603876000	5.083810000
H	-3.780794000	-0.095549000	5.743423000
H	-2.027366000	-0.348465000	5.713435000
C	-5.818073000	-0.348650000	-3.071938000
C	-2.943000000	0.130310000	3.755959000
H	-2.718362000	1.200985000	3.871434000
C	-4.332284000	-0.010296000	3.103519000
H	-4.322584000	0.317010000	2.057419000
H	-5.072551000	0.592526000	3.650734000
H	-4.660644000	-1.057958000	3.124208000
C	-0.210107000	-0.999286000	3.671861000
H	-0.677212000	-1.580555000	4.481651000
C	-2.510838000	2.865034000	-2.595361000
H	-3.389669000	3.405835000	-2.986104000
C	-4.500420000	3.160149000	-0.470389000
H	-5.185208000	3.159770000	-1.333807000
C	-4.059375000	4.613779000	-0.214461000
H	-3.273602000	4.673163000	0.549758000
H	-4.921091000	5.193993000	0.149117000

H	-3.694488000	5.103270000	-1.125187000
C	0.841364000	-1.884564000	2.982878000
H	0.393699000	-2.782562000	2.539803000
H	1.589379000	-2.202574000	3.726458000
H	1.353088000	-1.335003000	2.184992000
C	0.445845000	0.254093000	4.285439000
H	0.940250000	0.843828000	3.504284000
H	1.208612000	-0.044710000	5.020108000
H	-0.277875000	0.902160000	4.799504000
C	-5.256257000	2.596294000	0.742253000
H	-5.606000000	1.572614000	0.560014000
H	-6.134645000	3.224151000	0.955872000
H	-4.618662000	2.590651000	1.635440000
C	-2.015376000	1.869074000	-3.662696000
H	-1.164542000	1.290034000	-3.278499000
H	-1.671058000	2.427666000	-4.546716000
H	-2.800187000	1.172876000	-3.980442000
C	-1.384597000	3.868679000	-2.279939000
H	-1.666587000	4.614921000	-1.527432000
H	-1.098230000	4.405326000	-3.197302000
H	-0.507492000	3.322568000	-1.912086000
H	-3.181294000	-5.268499000	2.923065000
H	-3.349868000	-3.634538000	-1.902601000
H	-4.985800000	-3.922726000	-1.310250000
H	-6.609184000	-0.198689000	-3.805095000
H	0.366101000	1.059823000	0.883342000
H	-0.204715000	1.152074000	-1.171367000
Ti	1.353683000	0.297051000	-0.503116000
P	1.650068000	-1.804441000	-1.942905000
P	2.779794000	2.440255000	-0.273851000
N	3.107524000	-0.527399000	0.271153000
C	4.140059000	0.262997000	0.838672000
C	5.320825000	2.406218000	1.017317000
H	5.381917000	3.467868000	0.774808000
C	3.958771000	-4.693821000	-0.031020000
C	3.383079000	-1.919195000	0.209276000
C	5.126363000	-0.302294000	1.695197000
C	4.296675000	-2.551667000	1.091127000
C	4.579183000	-3.916358000	0.954453000
H	5.289878000	-4.375496000	1.643599000
C	4.917434000	-1.716758000	2.184441000
C	2.764806000	-2.708527000	-0.801295000
C	3.049628000	-4.081394000	-0.901824000
H	2.567677000	-4.674751000	-1.678597000
C	6.214717000	0.465149000	2.123826000
H	6.966841000	-0.004332000	2.760083000
C	4.222120000	1.657220000	0.558032000
C	2.726401000	-2.828902000	-4.465528000
H	3.135258000	-3.713797000	-3.956567000
H	3.386913000	-2.608240000	-5.317994000
H	1.739387000	-3.085294000	-4.871381000
C	6.339051000	1.815966000	1.773107000
C	2.690570000	-1.610418000	-3.524614000
H	2.212126000	-0.762829000	-4.038101000
C	4.125281000	-1.199027000	-3.139077000
H	4.124270000	-0.402598000	-2.386365000
H	4.662565000	-0.840622000	-4.029901000
H	4.675175000	-2.056565000	-2.728572000
C	0.333791000	-3.058540000	-2.423438000
H	0.845025000	-3.846753000	-2.997271000
C	2.465162000	3.881036000	0.927959000
H	3.412325000	4.443705000	0.968578000
C	3.497636000	3.372978000	-1.768943000
H	3.903581000	4.311116000	-1.354108000
C	2.404027000	3.705562000	-2.803107000
H	1.939698000	2.778464000	-3.164422000
H	2.855275000	4.230122000	-3.659336000
H	1.614128000	4.346063000	-2.395388000
C	-0.329249000	-3.698540000	-1.193058000
H	0.393969000	-4.252230000	-0.582754000
H	-1.108972000	-4.403117000	-1.519822000
H	-0.792689000	-2.935924000	-0.558929000
C	-0.705798000	-2.378888000	-3.339155000
H	-1.240675000	-1.591198000	-2.793257000
H	-1.443247000	-3.119095000	-3.684462000
H	-0.245939000	-1.924713000	-4.228242000
C	4.638554000	2.603613000	-2.458038000
H	5.450346000	2.349462000	-1.766508000
H	5.053197000	3.222142000	-3.268711000
H	4.256199000	1.676939000	-2.901473000
C	2.143620000	3.356934000	2.337485000
H	1.226686000	2.755986000	2.319603000
H	1.988771000	4.203180000	3.024256000
H	2.956743000	2.737358000	2.735366000
C	1.357260000	4.828452000	0.431360000
H	1.629134000	5.331827000	-0.504863000
H	1.175885000	5.609282000	1.185767000
H	0.416896000	4.285282000	0.273965000
H	4.183463000	-5.755513000	-0.122513000
H	4.242494000	-1.698021000	3.061647000
H	5.862940000	-2.158869000	2.529892000
H	7.194815000	2.401104000	2.106383000
H	1.993960000	0.779719000	-2.061218000
H	0.074392000	-0.895099000	0.209361000
N	-1.780870000	3.735621000	3.259147000
N	-1.526847000	3.335914000	2.247206000

TS_{DE}(open-shell singlet)

Ti	-1.335642000	0.443309000	0.225553000
P	-1.413391000	-0.492586000	2.618862000
P	-3.132137000	1.928636000	-1.136571000
N	-2.937752000	-0.864894000	0.087376000
C	-3.852897000	-0.790350000	-0.997402000
C	-4.988200000	0.524606000	-2.740270000
H	-5.124141000	1.475625000	-3.257058000
C	-3.522023000	-4.068359000	2.847513000
C	-3.116787000	-1.956137000	0.980135000
C	-4.606909000	-1.917663000	-1.428651000
C	-3.870772000	-3.106074000	0.629839000
C	-4.084831000	-4.123983000	1.568114000
H	-4.680438000	-4.988954000	1.271805000
C	-4.345142000	-3.261264000	-0.794088000
C	-2.519356000	-1.914788000	2.272723000
C	-2.719330000	-2.971290000	3.179135000
H	-2.235163000	-2.939836000	4.154004000
C	-5.541601000	-1.795365000	-2.462557000
H	-6.110985000	-2.679248000	-2.754512000
C	-4.062674000	0.443618000	-1.682788000
C	-2.273348000	-0.210386000	5.417894000
H	-2.824711000	-1.159906000	5.401798000
H	-2.781921000	0.452530000	6.134570000
H	-1.263092000	-0.397423000	5.803227000
C	-5.742019000	-0.583134000	-3.133823000
C	-2.266186000	0.456724000	4.029890000
H	-1.689081000	1.391169000	4.101114000
C	-3.701112000	0.800096000	3.588962000
H	-3.717305000	1.224273000	2.577166000
H	-4.151190000	1.528199000	4.279921000
H	-4.328960000	-0.101190000	3.580840000
C	0.071863000	-1.284238000	3.469079000
H	-0.326519000	-1.759844000	4.379034000
C	-2.495060000	2.724680000	-2.736085000
H	-3.362087000	3.234717000	-3.189604000
C	-4.594044000	3.070034000	-0.696865000
H	-5.259420000	2.974541000	-1.570285000
C	-4.225692000	4.556516000	-0.535792000
H	-3.478867000	4.709106000	0.254056000
H	-5.126885000	5.121721000	-0.254329000

H	-3.840381000	4.991993000	-1.465525000
C	0.726797000	-2.372325000	2.600596000
H	0.014840000	-3.163105000	2.334084000
H	1.556196000	-2.831458000	3.159590000
H	1.129227000	-1.944997000	1.675488000
C	1.096361000	-0.209410000	3.880316000
H	1.520761000	0.272132000	2.991622000
H	1.918396000	-0.678692000	4.441086000
H	0.657240000	0.569245000	4.520195000
C	-5.349618000	2.551783000	0.539017000
H	-5.580016000	1.481793000	0.460481000
H	-6.297992000	3.098854000	0.646914000
H	-4.765204000	2.715463000	1.452827000
C	-1.936871000	1.691114000	-3.733966000
H	-1.089107000	1.152645000	-3.290459000
H	-1.572911000	2.218747000	-4.628628000
H	-2.692753000	0.962047000	-4.048233000
C	-1.399858000	3.761313000	-2.407768000
H	-1.725625000	4.520960000	-1.686370000
H	-1.096470000	4.279179000	-3.329899000
H	-0.522880000	3.247207000	-1.996259000
H	-3.685819000	-4.872718000	3.562895000
H	-3.566374000	-3.790443000	-1.375140000
H	-5.243419000	-3.894323000	-0.841206000
H	-6.464615000	-0.506915000	-3.944605000
H	0.315032000	1.020229000	0.886980000
H	-0.328291000	1.094089000	-1.135485000
Ti	1.370144000	0.319330000	-0.574342000
P	1.585620000	-1.752217000	-2.056374000
P	2.792937000	2.432923000	-0.170155000
N	3.138915000	-0.552426000	0.168645000
C	4.152335000	0.198373000	0.818387000
C	5.289474000	2.341567000	1.205037000
H	5.334897000	3.420350000	1.050036000
C	4.018478000	-4.696981000	-0.404908000
C	3.425136000	-1.935000000	0.009606000
C	5.141386000	-0.416226000	1.638316000
C	4.354140000	-2.621129000	0.838198000
C	4.648540000	-3.971292000	0.612865000
H	5.373708000	-4.462670000	1.264154000
C	4.963597000	-1.871605000	1.997240000
C	2.785281000	-2.679713000	-1.025257000
C	3.079991000	-4.041961000	-1.210434000
H	2.574395000	-4.595099000	-2.002033000
C	6.204098000	0.332035000	2.156256000
H	6.954926000	-0.178310000	2.762320000
C	4.217956000	1.613587000	0.657177000
C	2.440500000	-2.761990000	-4.674487000
H	2.912077000	-3.642004000	-4.214029000
H	3.010406000	-2.526368000	-5.586510000
H	1.423014000	-3.034370000	-4.983521000
C	6.304446000	1.710922000	1.932097000
C	2.476270000	-1.549041000	-3.726449000
H	1.945846000	-0.703946000	-4.191330000
C	3.934226000	-1.120078000	-3.469690000
H	3.982802000	-0.314520000	-2.728257000
H	4.389504000	-0.764593000	-4.406446000
H	4.527090000	-1.966790000	-3.098067000
C	0.224060000	-3.003904000	-2.430927000
H	0.681061000	-3.801566000	-3.036730000
C	2.443698000	3.828026000	1.075390000
H	3.389938000	4.383276000	1.182026000
C	3.563299000	3.434803000	-1.596519000
H	3.954030000	4.356533000	-1.132324000
C	2.504228000	3.806284000	-2.653278000
H	2.068217000	2.890827000	-3.074921000
H	2.977104000	4.379892000	-3.465600000
H	1.689596000	4.414516000	-2.242712000
C	-0.360756000	-3.638657000	-1.156854000
H	0.407265000	-4.160402000	-0.572891000
H	-1.133903000	-4.371951000	-1.435466000
H	-0.819087000	-2.876673000	-0.515946000
C	-0.877528000	-2.319920000	-3.266225000
H	-1.353034000	-1.517877000	-2.686963000
H	-1.653804000	-3.050452000	-3.540653000
H	-0.485776000	-1.881183000	-4.194670000
C	4.729008000	2.692593000	-2.274700000
H	5.527625000	2.437655000	-1.568356000
H	5.154367000	3.328681000	-3.066351000
H	4.369207000	1.767429000	-2.740486000
C	2.057457000	3.256203000	2.450033000
H	1.148310000	2.647092000	2.373062000
H	1.867556000	4.078250000	3.157903000
H	2.857510000	2.628590000	2.861795000
C	1.369687000	4.805031000	0.559805000
H	1.708001000	5.360608000	-0.323791000
H	1.131189000	5.541927000	1.342409000
H	0.444727000	4.273883000	0.299898000
H	4.250679000	-5.749112000	-0.564215000
H	4.292434000	-1.947370000	2.875604000
H	5.919078000	-2.323609000	2.301160000
H	7.140199000	2.282202000	2.333732000
H	2.043220000	0.865540000	-2.119071000
H	-0.041449000	-0.831952000	0.006366000
N	-1.861389000	3.891013000	2.836229000
N	-1.627585000	3.332146000	1.898136000

TS_{DE}(triplet)

Ti	-1.228066000	0.483075000	0.217885000
P	-1.845014000	-0.369779000	2.625165000
P	-2.766270000	2.024241000	-1.235696000
N	-2.883474000	-0.783525000	-0.128359000
C	-3.806008000	-0.579898000	-1.174432000
C	-4.909592000	0.937338000	-2.759534000
H	-4.993613000	1.927846000	-3.209050000
C	-3.539208000	-4.155669000	2.393798000
C	-3.126793000	-1.903532000	0.696027000
C	-4.644966000	-1.624523000	-1.657358000
C	-3.881102000	-3.024502000	0.254837000
C	-4.086510000	-4.117400000	1.104341000
H	-4.669628000	-4.963388000	0.735962000
C	-4.392101000	-3.031820000	-1.167216000
C	-2.619086000	-1.921076000	2.031012000
C	-2.808734000	-3.052016000	2.847147000
H	-2.392525000	-3.063813000	3.854192000
C	-5.619744000	-1.359296000	-2.623989000
H	-6.256915000	-2.178134000	-2.963081000
C	-3.936691000	0.711215000	-1.767217000
C	-3.405855000	-0.323850000	5.108102000
H	-3.669419000	-1.382635000	4.979178000
H	-4.237966000	0.159946000	5.642493000
H	-2.519406000	-0.259583000	5.752022000
C	-5.770296000	-0.080602000	-3.179992000
C	-3.207496000	0.365754000	3.745642000
H	-2.887793000	1.404097000	3.920767000
C	-4.537055000	0.387105000	2.965343000
H	-4.407748000	0.777335000	1.949500000
H	-5.271800000	1.015454000	3.490624000
H	-4.949051000	-0.627316000	2.883592000
C	-0.529587000	-0.909839000	3.864254000
H	-1.048162000	-1.479351000	4.650796000
C	-2.039605000	2.681904000	-2.872927000
H	-2.804954000	3.362020000	-3.284476000
C	-3.977286000	3.443995000	-0.832593000
H	-4.628772000	3.519336000	-1.718550000
C	-3.285763000	4.805579000	-0.630411000
H	-2.516539000	4.755808000	0.152181000
H	-4.030197000	5.554262000	-0.319160000

H	-2.815356000	5.171488000	-1.551170000
C	0.535091000	-1.820768000	3.226434000
H	0.088697000	-2.721501000	2.787199000
H	1.254442000	-2.134004000	3.999461000
H	1.079566000	-1.296250000	2.432179000
C	0.121447000	0.331267000	4.508600000
H	0.649938000	0.924455000	3.751326000
H	0.855623000	0.018486000	5.265963000
H	-0.612640000	0.982272000	5.003929000
C	-4.855352000	3.088711000	0.378123000
H	-5.378662000	2.135931000	0.229109000
H	-5.611023000	3.873331000	0.536067000
H	-4.253225000	3.012993000	1.293296000
C	-1.754695000	1.571450000	-3.901330000
H	-1.005393000	0.874629000	-3.505821000
H	-1.348022000	2.026663000	-4.817880000
H	-2.655116000	1.006320000	-4.167943000
C	-0.741689000	3.469214000	-2.608197000
H	-0.874743000	4.290555000	-1.893515000
H	-0.370386000	3.898345000	-3.551790000
H	0.024921000	2.789201000	-2.213677000
H	-3.687673000	-5.023644000	3.034566000
H	-3.637195000	-3.508349000	-1.821937000
H	-5.300477000	-3.646528000	-1.252889000
H	-6.530246000	0.110628000	-3.936271000
H	0.445707000	1.360459000	0.562572000
H	-0.209128000	0.520713000	-1.384295000
Ti	1.434951000	0.276182000	-0.510058000
P	1.545916000	-1.834077000	-1.951101000
P	3.027610000	2.305010000	-0.196002000
N	3.115370000	-0.676640000	0.281850000
C	4.138528000	0.027400000	0.968880000
C	5.392339000	2.103783000	1.368231000
H	5.516069000	3.172682000	1.189928000
C	3.801313000	-4.859877000	-0.204822000
C	3.321471000	-2.077624000	0.162121000
C	5.030099000	-0.627802000	1.864422000
C	4.168790000	-2.795280000	1.046380000
C	4.411720000	-4.158750000	0.842086000
H	5.077132000	-4.679848000	1.532309000
C	4.742579000	-2.062652000	2.234146000
C	2.686548000	-2.797055000	-0.889012000
C	2.927576000	-4.172408000	-1.054311000
H	2.426801000	-4.710800000	-1.858525000
C	6.104846000	0.066818000	2.429536000
H	6.781887000	-0.472717000	3.093811000
C	4.316411000	1.426340000	0.766133000
C	2.371648000	-2.907787000	-4.546731000
H	2.814389000	-3.795608000	-4.073075000
H	2.949308000	-2.703522000	-5.461176000
H	1.346004000	-3.150503000	-4.851940000
C	6.309638000	1.430386000	2.180271000
C	2.445999000	-1.681655000	-3.617688000
H	1.943027000	-0.828123000	-4.097102000
C	3.915526000	-1.297001000	-3.360567000
H	3.985490000	-0.480061000	-2.633264000
H	4.388605000	-0.973539000	-4.299804000
H	4.478462000	-2.154905000	-2.968740000
C	0.134701000	-3.026006000	-2.307910000
H	0.570418000	-3.852401000	-2.891096000
C	2.633999000	3.751835000	0.965844000
H	3.571186000	4.326111000	1.055077000
C	3.949704000	3.190512000	-1.606061000
H	4.331056000	4.121326000	-1.153390000
C	3.002872000	3.547087000	-2.768938000
H	2.571240000	2.632922000	-3.196279000
H	3.568729000	4.071669000	-3.553810000
H	2.176621000	4.196843000	-2.458286000
C	-0.470226000	-3.603316000	-1.017232000
H	0.267118000	-4.181399000	-0.447000000
H	-1.306858000	-4.271401000	-1.270553000
H	-0.850463000	-2.803794000	-0.372634000
C	-0.932197000	-2.321962000	-3.169641000
H	-1.392627000	-1.498221000	-2.611329000
H	-1.721912000	-3.037283000	-3.443755000
H	-0.514466000	-1.912600000	-4.100284000
C	5.146146000	2.377002000	-2.133570000
H	5.871026000	2.142441000	-1.345831000
H	5.658559000	2.956989000	-2.915992000
H	4.807774000	1.435547000	-2.582090000
C	2.227329000	3.246612000	2.361333000
H	1.329559000	2.620141000	2.290973000
H	2.000122000	4.104252000	3.012760000
H	3.026153000	2.660611000	2.831508000
C	1.545214000	4.671591000	0.381536000
H	1.855569000	5.140233000	-0.560778000
H	1.322776000	5.478801000	1.095858000
H	0.620931000	4.107603000	0.202375000
H	3.993093000	-5.922223000	-0.347912000
H	4.009396000	-2.082892000	3.063395000
H	5.647487000	-2.562609000	2.608101000
H	7.151497000	1.957918000	2.625816000
H	2.000219000	0.712494000	-2.098450000
H	0.181408000	-0.808916000	0.333392000
N	-1.736976000	4.021238000	3.188891000
N	-1.392972000	3.330145000	2.382937000

E(closed-shell singlet)

Ti	-1.281551000	0.630539000	0.484335000
P	-1.331878000	-0.690245000	2.647810000
P	-2.873215000	2.053420000	-1.022947000
N	-2.955803000	-0.696974000	0.137534000
C	-3.921461000	-0.506256000	-0.894188000
C	-5.066193000	1.001999000	-2.478888000
H	-5.145546000	1.991128000	-2.932768000
C	-3.511877000	-4.208384000	2.551268000
C	-3.128820000	-1.885084000	0.906394000
C	-4.782522000	-1.542057000	-1.358865000
C	-3.953119000	-2.968748000	0.489934000
C	-4.149040000	-4.084991000	1.313364000
H	-4.799482000	-4.883977000	0.952974000
C	-4.552450000	-2.954204000	-0.891152000
C	-2.471034000	-2.030225000	2.166213000
C	-2.658778000	-3.178048000	2.956717000
H	-2.128546000	-3.264272000	3.904544000
C	-5.781385000	-1.277451000	-2.304016000
H	-6.427331000	-2.100658000	-2.614693000
C	-4.066874000	0.766405000	-1.520034000
C	-2.167999000	-0.594412000	5.461076000
H	-2.685448000	-1.560515000	5.382091000
H	-2.698489000	0.000831000	6.220243000
H	-1.151532000	-0.772404000	5.835160000
C	-5.948918000	-0.008685000	-2.869195000
C	-2.186632000	0.160521000	4.119078000
H	-1.634403000	1.105556000	4.236723000
C	-3.635404000	0.499113000	3.715829000
H	-3.679863000	0.974873000	2.728538000
H	-4.081842000	1.185563000	4.450319000
H	-4.248535000	-0.411379000	3.675811000
C	0.132044000	-1.568588000	3.445998000
H	-0.276242000	-2.116490000	4.309482000
C	-2.252951000	2.777904000	-2.661036000
H	-3.102017000	3.353405000	-3.068165000
C	-4.086311000	3.393316000	-0.421136000
H	-4.802269000	3.477235000	-1.255424000
C	-3.468081000	4.783473000	-0.177505000
H	-2.648036000	4.744949000	0.550359000
H	-4.242245000	5.452380000	0.228493000

H	-3.096059000	5.237729000	-1.103619000
C	0.788290000	-2.583196000	2.494169000
H	0.073498000	-3.342486000	2.154208000
H	1.610897000	-3.095276000	3.017209000
H	1.201169000	-2.079286000	1.612203000
C	1.161989000	-0.542946000	3.960137000
H	1.603258000	0.011206000	3.122929000
H	1.972689000	-1.064964000	4.490385000
H	0.719713000	0.183481000	4.655993000
C	-4.861946000	2.912571000	0.820386000
H	-5.280486000	1.908254000	0.677247000
H	-5.694135000	3.604018000	1.021037000
H	-4.218521000	2.901810000	1.707957000
C	-1.865299000	1.672837000	-3.662219000
H	-1.031454000	1.082290000	-3.260612000
H	-1.532232000	2.138063000	-4.602802000
H	-2.700961000	0.999786000	-3.886576000
C	-1.046964000	3.717604000	-2.455940000
H	-1.241620000	4.522701000	-1.738448000
H	-0.782490000	4.179603000	-3.419603000
H	-0.186577000	3.139930000	-2.098952000
H	-3.666364000	-5.086363000	3.176608000
H	-3.861595000	-3.460797000	-1.593108000
H	-5.487328000	-3.533830000	-0.918033000
H	-6.726618000	0.178320000	-3.607976000
H	0.476255000	0.892183000	1.096738000
H	-0.213970000	1.355785000	-0.805442000
Ti	1.310760000	0.341545000	-0.463511000
P	1.316266000	-1.515485000	-2.238664000
P	2.844370000	2.338034000	0.105277000
N	3.077081000	-0.654391000	0.027027000
C	4.077652000	-0.051987000	0.842039000
C	5.167303000	1.970959000	1.713855000
H	5.208113000	3.058405000	1.781698000
C	3.963604000	-4.596249000	-1.364476000
C	3.351558000	-1.984808000	-0.394895000
C	5.039811000	-0.820518000	1.551884000
C	4.302359000	-2.808485000	0.265061000
C	4.612514000	-4.077760000	-0.238577000
H	5.360725000	-4.676614000	0.283327000
C	4.904927000	-2.323126000	1.560324000
C	2.666626000	-2.530179000	-1.520335000
C	2.973433000	-3.823320000	-1.980217000
H	2.428804000	-4.232079000	-2.830348000
C	6.057103000	-0.189807000	2.278143000
H	6.787951000	-0.811933000	2.797404000
C	4.147312000	1.366361000	0.958426000
C	1.802047000	-2.181754000	-5.046261000
H	2.458930000	-3.023619000	-4.787377000
H	2.142878000	-1.788678000	-6.016092000
H	0.783079000	-2.563726000	-5.185703000
C	6.138596000	1.204736000	2.365720000
C	1.886669000	-1.060529000	-3.992895000
H	1.200225000	-0.247238000	-4.275168000
C	3.314092000	-0.486007000	-3.939183000
H	3.378514000	0.317871000	-3.197871000
H	3.588936000	-0.077745000	-4.923283000
H	4.040563000	-1.266540000	-3.674874000
C	-0.058982000	-2.773003000	-2.525761000
H	0.346016000	-3.510210000	-3.236549000
C	2.459256000	3.705729000	1.355988000
H	3.397104000	4.273216000	1.478768000
C	3.794977000	3.321907000	-1.225220000
H	4.157238000	4.220442000	-0.697930000
C	2.881343000	3.762258000	-2.385220000
H	2.484771000	2.885257000	-2.911687000
H	3.460705000	4.371600000	-3.095713000
H	2.027916000	4.360178000	-2.044456000
C	-0.448423000	-3.507244000	-1.230690000
H	0.403359000	-4.047691000	-0.799471000
H	-1.240898000	-4.238691000	-1.450601000
H	-0.828458000	-2.802743000	-0.482299000
C	-1.278987000	-2.083835000	-3.165695000
H	-1.707908000	-1.347819000	-2.475384000
H	-2.052893000	-2.832525000	-3.391640000
H	-1.027851000	-1.570225000	-4.103895000
C	5.016778000	2.552659000	-1.763795000
H	5.752826000	2.347263000	-0.978409000
H	5.504385000	3.150845000	-2.548444000
H	4.718513000	1.595007000	-2.207672000
C	2.052578000	3.130244000	2.723970000
H	1.170239000	2.488183000	2.631251000
H	1.806364000	3.954636000	3.409795000
H	2.863404000	2.541617000	3.170445000
C	1.384332000	4.662628000	0.801801000
H	1.742190000	5.213987000	-0.077299000
H	1.115684000	5.400428000	1.571961000
H	0.477027000	4.113509000	0.523619000
H	4.208847000	-5.587957000	-1.741337000
H	4.248644000	-2.624482000	2.399424000
H	5.877156000	-2.802743000	1.745110000
H	6.933551000	1.681827000	2.936773000
H	1.679278000	1.091916000	-1.979910000
H	-0.103463000	-0.740381000	0.069835000
N	-1.489685000	3.187305000	2.353160000
N	-1.390725000	2.295398000	1.636623000

E(open-shell singlet)

Ti	-1.294256000	0.640848000	0.482348000
P	-1.376262000	-0.742815000	2.645069000
P	-2.866645000	2.104244000	-0.988235000
N	-2.968810000	-0.686283000	0.104276000
C	-3.883588000	-0.481039000	-0.964762000
C	-4.941843000	1.047516000	-2.590924000
H	-4.997549000	2.042479000	-3.035456000
C	-3.676791000	-4.176642000	2.502141000
C	-3.182048000	-1.869020000	0.863494000
C	-4.735702000	-1.504952000	-1.471727000
C	-4.016637000	-2.936343000	0.421336000
C	-4.270988000	-4.040634000	1.243151000
H	-4.930849000	-4.823684000	0.865258000
C	-4.553628000	-2.918201000	-0.985761000
C	-2.553717000	-2.036346000	2.135868000
C	-2.799052000	-3.175144000	2.924592000
H	-2.288704000	-3.278923000	3.881517000
C	-5.682033000	-1.227752000	-2.465131000
H	-6.321565000	-2.042570000	-2.809355000
C	-3.995637000	0.800558000	-1.581064000
C	-2.110613000	-0.686283000	5.485643000
H	-2.649920000	-1.640802000	5.416363000
H	-2.596953000	-0.091755000	6.274135000
H	-1.082879000	-0.888621000	5.813085000
C	-5.806519000	0.044386000	-3.035253000
C	-2.172038000	0.090998000	4.157319000
H	-1.605577000	1.027523000	4.273807000
C	-3.631763000	0.449245000	3.813686000
H	-3.709188000	0.948755000	2.840521000
H	-4.045495000	1.120349000	4.580696000
H	-4.252214000	-0.456104000	3.774307000
C	0.084006000	-1.688677000	3.369437000
H	-0.312716000	-2.247542000	4.231493000
C	-2.216099000	2.945185000	-2.556860000
H	-3.061871000	3.532768000	-2.953117000
C	-4.147831000	3.365763000	-0.358596000
H	-4.857410000	3.446448000	-1.198678000
C	-3.597427000	4.772571000	-0.056077000
H	-2.787892000	4.744675000	0.684187000
H	-4.406570000	5.392260000	0.359602000

H	-3.230296000	5.275540000	-0.958854000
C	0.668657000	-2.695466000	2.364029000
H	-0.081478000	-3.427505000	2.040893000
H	1.500685000	-3.240695000	2.835489000
H	1.052885000	-2.180221000	1.475600000
C	1.164827000	-0.709854000	3.868805000
H	1.594560000	-0.153175000	3.027340000
H	1.975173000	-1.270247000	4.358848000
H	0.772554000	0.015698000	4.595124000
C	-4.909804000	2.801631000	0.855439000
H	-5.273384000	1.782472000	0.672510000
H	-5.778596000	3.440966000	1.072899000
H	-4.272788000	2.791498000	1.747898000
C	-1.767920000	1.922092000	-3.618026000
H	-0.932951000	1.322907000	-3.231817000
H	-1.415505000	2.460519000	-4.511238000
H	-2.579048000	1.248623000	-3.918298000
C	-1.039373000	3.890244000	-2.237537000
H	-1.280948000	4.641448000	-1.476719000
H	-0.740993000	4.420919000	-3.154579000
H	-0.184055000	3.302966000	-1.883343000
H	-3.875330000	-5.047344000	3.125047000
H	-3.840653000	-3.442205000	-1.651814000
H	-5.497128000	-3.480365000	-1.052279000
H	-6.543272000	0.241208000	-3.812412000
H	0.480752000	0.911977000	1.050169000
H	-0.253756000	1.313298000	-0.867533000
Ti	1.327033000	0.358847000	-0.494917000
P	1.337237000	-1.480110000	-2.281894000
P	2.885716000	2.328105000	0.156049000
N	3.070376000	-0.672461000	0.030931000
C	4.096337000	-0.092023000	0.827922000
C	5.266397000	1.903518000	1.658161000
H	5.339942000	2.989925000	1.716794000
C	3.820168000	-4.662319000	-1.307803000
C	3.301209000	-2.014866000	-0.376324000
C	5.044447000	-0.882616000	1.533833000
C	4.220190000	-2.864544000	0.296486000
C	4.483249000	-4.152203000	-0.186195000
H	5.206534000	-4.770748000	0.347788000
C	4.845890000	-2.377316000	1.579600000
C	2.610011000	-2.547357000	-1.504818000
C	2.869477000	-3.858020000	-1.944688000
H	2.321076000	-4.253519000	-2.798876000
C	6.099129000	-0.277816000	2.227607000
H	6.817925000	-0.917786000	2.742082000
C	4.207898000	1.323991000	0.936725000
C	1.933064000	-2.134915000	-5.072931000
H	2.506708000	-3.026919000	-4.784790000
H	2.366979000	-1.757040000	-6.011195000
H	0.900353000	-2.438122000	-5.286543000
C	6.231722000	1.114312000	2.291221000
C	2.026592000	-1.037170000	-3.996445000
H	1.409612000	-0.177159000	-4.300125000
C	3.481717000	-0.555525000	-3.848053000
H	3.557761000	0.207189000	-3.065142000
H	3.830505000	-0.120757000	-4.796690000
H	4.144990000	-1.391252000	-3.586765000
C	-0.074851000	-2.669653000	-2.659323000
H	0.323892000	-3.401772000	-3.378718000
C	2.526455000	3.615311000	1.499388000
H	3.475804000	4.154106000	1.656823000
C	3.796970000	3.399396000	-1.132485000
H	4.177402000	4.262036000	-0.559677000
C	2.846354000	3.909984000	-2.232685000
H	2.424016000	3.063568000	-2.788849000
H	3.405439000	4.551495000	-2.931060000
H	2.012261000	4.496632000	-1.830214000
C	-0.549295000	-3.426363000	-1.406446000
H	0.260805000	-4.011370000	-0.953874000
H	-1.356649000	-4.120643000	-1.685311000
H	-0.936487000	-2.730457000	-0.653919000
C	-1.236346000	-1.904742000	-3.323260000
H	-1.654598000	-1.165270000	-2.629891000
H	-2.038483000	-2.606551000	-3.596101000
H	-0.925219000	-1.380741000	-4.237647000
C	4.997312000	2.669840000	-1.764651000
H	5.745649000	2.379390000	-1.018720000
H	5.478195000	3.333788000	-2.499008000
H	4.672608000	1.765281000	-2.292780000
C	2.115490000	2.951614000	2.825179000
H	1.209668000	2.349511000	2.694343000
H	1.906574000	3.729076000	3.575421000
H	2.910085000	2.303032000	3.214194000
C	1.466841000	4.630944000	1.027712000
H	1.825149000	5.237616000	0.186249000
H	1.221596000	5.316709000	1.852107000
H	0.543889000	4.123222000	0.723016000
H	4.028243000	-5.668510000	-1.668354000
H	4.178704000	-2.628283000	2.426993000
H	5.796506000	-2.894608000	1.774659000
H	7.056688000	1.571861000	2.835052000
H	1.763684000	1.134300000	-1.990641000
H	-0.095828000	-0.727513000	-0.019192000
N	-1.508025000	3.115982000	2.471590000
N	-1.427831000	2.257093000	1.716526000

E(triplet)

Ti	-1.284202000	0.701830000	0.473539000
P	-1.524190000	-0.583949000	2.710904000
P	-2.839845000	1.979658000	-1.196495000
N	-2.917984000	-0.764302000	0.080252000
C	-3.809915000	-0.630608000	-1.003491000
C	-4.934005000	0.801694000	-2.673365000
H	-5.027983000	1.776670000	-3.154177000
C	-3.465194000	-4.231564000	2.543219000
C	-3.081762000	-1.928921000	0.860985000
C	-4.609883000	-1.708984000	-1.494661000
C	-3.825193000	-3.066469000	0.421769000
C	-4.024198000	-4.167070000	1.260605000
H	-4.611855000	-5.005246000	0.881030000
C	-4.326070000	-3.102655000	-0.998491000
C	-2.506491000	-2.014138000	2.167354000
C	-2.693539000	-3.151005000	2.976180000
H	-2.224092000	-3.188505000	3.958927000
C	-5.578157000	-1.498310000	-2.479750000
H	-6.179087000	-2.350214000	-2.803923000
C	-3.968136000	0.625012000	-1.664821000
C	-2.602747000	-0.517343000	5.426566000
H	-3.057499000	-1.510637000	5.311315000
H	-3.226086000	0.049753000	6.134751000
H	-1.611707000	-0.637156000	5.883149000
C	-5.767752000	-0.243471000	-3.074852000
C	-2.553522000	0.232026000	4.082057000
H	-2.071101000	1.208783000	4.239649000
C	-3.980719000	0.476412000	3.551138000
H	-3.971063000	0.963305000	2.568866000
H	-4.536033000	1.117294000	4.251851000
H	-4.521531000	-0.474114000	3.449181000
C	-0.056602000	-1.331389000	3.625003000
H	-0.470726000	-1.922255000	4.456731000
C	-2.181562000	2.580458000	-2.875047000
H	-3.037755000	3.062897000	-3.376534000
C	-4.098258000	3.334660000	-0.741515000
H	-4.753941000	3.396585000	-1.625989000
C	-3.499086000	4.732049000	-0.487870000
H	-2.724267000	4.708383000	0.288474000
H	-4.295547000	5.408161000	-0.141202000

H	-3.071027000	5.170749000	-1.397021000
C	0.742852000	-2.273191000	2.707949000
H	0.121863000	-3.093009000	2.327026000
H	1.584019000	-2.709016000	3.269142000
H	1.152304000	-1.721433000	1.851719000
C	0.845327000	-0.224585000	4.205652000
H	1.288427000	0.370385000	3.397616000
H	1.663743000	-0.677139000	4.785667000
H	0.297870000	0.455087000	4.873421000
C	-4.957873000	2.885078000	0.456248000
H	-5.376776000	1.882744000	0.302641000
H	-5.793156000	3.589031000	0.590512000
H	-4.371786000	2.882146000	1.382660000
C	-1.693329000	1.397659000	-3.733784000
H	-0.857677000	0.890225000	-3.231631000
H	-1.327276000	1.777796000	-4.700299000
H	-2.487579000	0.667618000	-3.927040000
C	-1.032471000	3.597135000	-2.730025000
H	-1.297586000	4.471043000	-2.124512000
H	-0.736751000	3.955986000	-3.728056000
H	-0.166211000	3.106724000	-2.270942000
H	-3.615079000	-5.103837000	3.177523000
H	-3.555070000	-3.567511000	-1.644647000
H	-5.217711000	-3.741568000	-1.085181000
H	-6.522993000	-0.095806000	-3.845237000
H	0.514930000	0.725719000	1.075562000
H	-0.068507000	1.470128000	-0.744260000
Ti	1.309289000	0.254506000	-0.524867000
P	1.576806000	-1.681261000	-2.184150000
P	2.682703000	2.397137000	0.012311000
N	3.096160000	-0.553241000	0.160241000
C	3.988265000	0.154384000	1.013885000
C	4.883827000	2.291925000	1.822242000
H	4.855103000	3.381791000	1.819439000
C	4.313101000	-4.516678000	-0.892637000
C	3.473833000	-1.889613000	-0.153598000
C	4.931547000	-0.508166000	1.842649000
C	4.410727000	-2.611066000	0.635019000
C	4.834562000	-3.886640000	0.242799000
H	5.570795000	-4.402221000	0.861424000
C	4.879692000	-2.012535000	1.938635000
C	2.919037000	-2.549535000	-1.291586000
C	3.334973000	-3.848634000	-1.635507000
H	2.883712000	-4.343704000	-2.494322000
C	5.849608000	0.230274000	2.599230000
H	6.570985000	-0.309526000	3.214657000
C	3.963413000	1.576067000	1.037209000
C	2.311179000	-2.508854000	-4.880433000
H	3.032144000	-3.251952000	-4.513300000
H	2.668903000	-2.162672000	-5.861707000
H	1.345736000	-3.005585000	-5.038154000
C	5.842724000	1.630092000	2.595800000
C	2.216000000	-1.302634000	-3.926851000
H	1.471278000	-0.591869000	-4.317561000
C	3.569359000	-0.575495000	-3.833499000
H	3.490647000	0.301274000	-3.181588000
H	3.881933000	-0.240694000	-4.833678000
H	4.346947000	-1.241507000	-3.434991000
C	0.267075000	-3.009325000	-2.442784000
H	0.733967000	-3.786760000	-3.067699000
C	2.116026000	3.824119000	1.119602000
H	2.995986000	4.481404000	1.223297000
C	3.701997000	3.330750000	-1.304721000
H	3.993989000	4.273667000	-0.812628000
C	2.873913000	3.665182000	-2.560340000
H	2.527078000	2.746051000	-3.048850000
H	3.498608000	4.228825000	-3.269919000
H	1.991759000	4.274167000	-2.331784000
C	-0.168314000	-3.646421000	-1.110577000
H	0.675600000	-4.115914000	-0.589776000
H	-0.921998000	-4.423049000	-1.308659000
H	-0.617268000	-2.897409000	-0.447670000
C	-0.938995000	-2.415627000	-3.197346000
H	-1.430314000	-1.645739000	-2.590063000
H	-1.672929000	-3.209007000	-3.401436000
H	-0.655684000	-1.968743000	-4.160459000
C	4.986729000	2.571539000	-1.691888000
H	5.670082000	2.461076000	-0.842565000
H	5.508818000	3.124871000	-2.487055000
H	4.758012000	1.569210000	-2.074232000
C	1.697461000	3.336126000	2.517648000
H	0.885171000	2.605703000	2.445930000
H	1.339020000	4.190923000	3.109879000
H	2.535172000	2.872466000	3.052300000
C	0.985895000	4.628223000	0.447279000
H	1.317798000	5.110869000	-0.480769000
H	0.641382000	5.417949000	1.130828000
H	0.133187000	3.978972000	0.216237000
H	4.644728000	-5.513419000	-1.178689000
H	4.176050000	-2.301648000	2.742529000
H	5.858880000	-2.421429000	2.226945000
H	6.560656000	2.191518000	3.191552000
H	1.639951000	1.001569000	-2.046472000
H	-0.220049000	-0.680045000	-0.343906000
N	-1.816666000	3.181533000	2.375143000
N	-1.650033000	2.292869000	1.663382000

TS_{EF}(closed-shell singlet)

Ti	-1.379191000	0.597689000	0.590456000
P	-1.454646000	-0.996831000	2.562243000
P	-2.912411000	2.212376000	-0.817782000
N	-3.011436000	-0.693925000	0.005932000
C	-3.931685000	-0.377597000	-1.028684000
C	-5.036479000	1.315873000	-2.447221000
H	-5.109148000	2.353747000	-2.776408000
C	-3.574329000	-4.493597000	1.926830000
C	-3.185591000	-1.970586000	0.610052000
C	-4.779901000	-1.346300000	-1.641048000
C	-3.991544000	-2.996432000	0.038776000
C	-4.192962000	-4.211391000	0.705102000
H	-4.831111000	-4.959983000	0.232029000
C	-4.561224000	-2.806165000	-1.342854000
C	-2.543909000	-2.277247000	1.850231000
C	-2.734934000	-3.521518000	2.477739000
H	-2.214334000	-3.730701000	3.411580000
C	-5.754637000	-0.965923000	-2.570681000
H	-6.392725000	-1.742820000	-2.995732000
C	-4.061287000	0.964753000	-1.497183000
C	-2.366680000	-1.326534000	5.333939000
H	-2.835454000	-2.293227000	5.104403000
H	-2.945983000	-0.865962000	6.148908000
H	-1.353705000	-1.510075000	5.714141000
C	-5.908535000	0.363392000	-2.980124000
C	-2.382374000	-0.391560000	4.110423000
H	-1.868899000	0.543904000	4.380994000
C	-3.834551000	-0.050510000	3.719214000
H	-3.880367000	0.566448000	2.813477000
H	-4.326413000	0.498321000	4.535989000
H	-4.407283000	-0.967227000	3.525177000
C	0.015863000	-1.940009000	3.276312000
H	-0.388512000	-2.588899000	4.068680000
C	-2.324765000	3.192881000	-2.332671000
H	-3.183196000	3.816696000	-2.635131000
C	-4.172434000	3.413342000	-0.042286000
H	-4.884113000	3.600991000	-0.863096000
C	-3.593422000	4.765650000	0.415514000
H	-2.778204000	4.637264000	1.139016000
H	-4.386809000	5.347073000	0.909183000

H	-3.224616000	5.364770000	-0.425639000
C	0.712304000	-2.828816000	2.231704000
H	0.022873000	-3.562305000	1.796302000
H	1.537632000	-3.375363000	2.713404000
H	1.130664000	-2.224115000	1.417642000
C	1.011025000	-0.946576000	3.908245000
H	1.434523000	-0.291007000	3.136494000
H	1.838173000	-1.496507000	4.381298000
H	0.544226000	-0.314712000	4.677154000
C	-4.941889000	2.731647000	1.105148000
H	-5.326733000	1.746934000	0.811445000
H	-5.796976000	3.360029000	1.395841000
H	-4.305210000	2.610547000	1.989772000
C	-1.941862000	2.273102000	-3.509240000
H	-1.117241000	1.605533000	-3.229576000
H	-1.604531000	2.891701000	-4.354847000
H	-2.784578000	1.658696000	-3.845379000
C	-1.136175000	4.111246000	-1.978186000
H	-1.351891000	4.792485000	-1.147568000
H	-0.874328000	4.721521000	-2.855959000
H	-0.260351000	3.512374000	-1.705022000
H	-3.728806000	-5.448678000	2.426402000
H	-3.855612000	-3.225633000	-2.086235000
H	-5.496149000	-3.374149000	-1.461708000
H	-6.669041000	0.642646000	-3.707463000
H	0.338550000	1.207709000	0.988536000
H	-0.084180000	1.300032000	-1.115284000
Ti	1.309762000	0.355774000	-0.324111000
P	1.372387000	-1.330067000	-2.285087000
P	2.958607000	2.299501000	0.295107000
N	3.171438000	-0.665365000	-0.006321000
C	4.200150000	-0.129656000	0.809357000
C	5.351782000	1.824158000	1.768434000
H	5.407002000	2.905282000	1.903460000
C	3.995735000	-4.501265000	-1.697539000
C	3.426356000	-1.958100000	-0.526682000
C	5.178725000	-0.949970000	1.440237000
C	4.384116000	-2.838168000	0.049446000
C	4.671885000	-4.069833000	-0.550098000
H	5.423158000	-4.711910000	-0.086637000
C	5.009919000	-2.447745000	1.366191000
C	2.717846000	-2.416061000	-1.678678000
C	3.004522000	-3.674811000	-2.237893000
H	2.441766000	-4.015098000	-3.106584000
C	6.229561000	-0.377520000	2.165253000
H	6.968047000	-1.039797000	2.620769000
C	4.297038000	1.278534000	1.014963000
C	2.139041000	-1.703788000	-5.083048000
H	2.893518000	-2.455859000	-4.815207000
H	2.483751000	-1.200981000	-5.999705000
H	1.200934000	-2.220701000	-5.323923000
C	6.335893000	1.008958000	2.336020000
C	1.973237000	-0.664789000	-3.959651000
H	1.191559000	0.056231000	-4.248481000
C	3.282766000	0.113408000	-3.739993000
H	3.154906000	0.869612000	-2.955313000
H	3.586907000	0.620751000	-4.667979000
H	4.093459000	-0.562448000	-3.434530000
C	0.004205000	-2.530449000	-2.767431000
H	0.425001000	-3.207593000	-3.526989000
C	2.571206000	3.513528000	1.695335000
H	3.502774000	4.076443000	1.873432000
C	3.840153000	3.463067000	-0.941559000
H	4.140936000	4.338206000	-0.341669000
C	2.878392000	3.937327000	-2.049142000
H	2.521075000	3.088759000	-2.646764000
H	3.399539000	4.638651000	-2.718793000
H	1.997456000	4.449027000	-1.643780000
C	-0.450086000	-3.370802000	-1.560788000
H	0.377514000	-3.961399000	-1.148389000
H	-1.244749000	-4.065813000	-1.872075000
H	-0.845584000	-2.727736000	-0.766461000
C	-1.173681000	-1.759038000	-3.393332000
H	-1.601245000	-1.054536000	-2.668681000
H	-1.965224000	-2.462925000	-3.691029000
H	-0.875768000	-1.197054000	-4.289536000
C	5.112267000	2.841584000	-1.550823000
H	5.861560000	2.610815000	-0.785584000
H	5.554461000	3.550877000	-2.267100000
H	4.889159000	1.913594000	-2.091548000
C	2.185745000	2.778677000	2.991443000
H	1.282318000	2.176736000	2.839081000
H	1.980609000	3.513627000	3.784543000
H	2.990662000	2.117327000	3.335056000
C	1.471989000	4.508369000	1.274159000
H	1.787188000	5.142534000	0.435132000
H	1.228865000	5.170637000	2.118451000
H	0.557904000	3.974665000	0.984017000
H	4.220891000	-5.467089000	-2.147399000
H	4.351060000	-2.780261000	2.192574000
H	5.971145000	-2.961180000	1.514952000
H	7.155884000	1.439577000	2.908709000
H	0.735137000	1.466859000	-1.642144000
H	-0.140097000	-0.693893000	0.193033000
N	-1.556016000	2.838990000	2.873342000
N	-1.486268000	2.058403000	2.043343000

TS_{EF}(quintet)

Ti	-1.329989000	0.673176000	0.544842000
P	-1.490843000	-0.939763000	2.558765000
P	-2.949616000	2.159703000	-0.845952000
N	-3.008636000	-0.765747000	-0.008628000
C	-3.912560000	-0.475001000	-1.040586000
C	-5.044436000	1.187431000	-2.467526000
H	-5.142399000	2.220641000	-2.803401000
C	-3.473785000	-4.529013000	1.961423000
C	-3.147751000	-2.023012000	0.606103000
C	-4.738279000	-1.469556000	-1.656639000
C	-3.918425000	-3.085160000	0.041637000
C	-4.085408000	-4.293518000	0.724272000
H	-4.691335000	-5.073065000	0.259110000
C	-4.478429000	-2.919527000	-1.345993000
C	-2.514365000	-2.281510000	1.863713000
C	-2.678557000	-3.517918000	2.510922000
H	-2.171402000	-3.694244000	3.458723000
C	-5.710635000	-1.116902000	-2.594556000
H	-6.327511000	-1.907109000	-3.026002000
C	-4.062758000	0.868337000	-1.513315000
C	-2.443849000	-1.264707000	5.312190000
H	-2.904503000	-2.236038000	5.085532000
H	-3.033081000	-0.802478000	6.118995000
H	-1.432921000	-1.439552000	5.702238000
C	-5.888623000	0.211543000	-3.004604000
C	-2.456227000	-0.338809000	4.082106000
H	-1.962838000	0.608285000	4.348765000
C	-3.905055000	-0.024387000	3.659599000
H	-3.936290000	0.587811000	2.750487000
H	-4.421177000	0.520956000	4.463506000
H	-4.459785000	-0.951560000	3.460815000
C	0.001127000	-1.823207000	3.297461000
H	-0.385599000	-2.504977000	4.071117000
C	-2.363374000	3.102458000	-2.388769000
H	-3.223547000	3.711566000	-2.715966000
C	-4.241113000	3.371263000	-0.140063000
H	-4.943281000	3.529317000	-0.975624000
C	-3.678349000	4.742770000	0.281171000
H	-2.875784000	4.641951000	1.022665000
H	-4.482921000	5.336911000	0.740926000

H	-3.297306000	5.314236000	-0.573894000
C	0.744098000	-2.655752000	2.238729000
H	0.098798000	-3.428186000	1.802634000
H	1.609701000	-3.152700000	2.703397000
H	1.108948000	-2.014523000	1.426481000
C	0.944416000	-0.802274000	3.964214000
H	1.354042000	-0.115806000	3.213155000
H	1.783159000	-1.329149000	4.443722000
H	0.438449000	-0.205556000	4.736132000
C	-5.017308000	2.721553000	1.020459000
H	-5.405322000	1.731452000	0.748820000
H	-5.871408000	3.359697000	1.293601000
H	-4.380877000	2.617330000	1.907005000
C	-1.953577000	2.151714000	-3.530230000
H	-1.120135000	1.512985000	-3.210587000
H	-1.613774000	2.747828000	-4.391416000
H	-2.781667000	1.513405000	-3.859431000
C	-1.179098000	4.034292000	-2.055517000
H	-1.394774000	4.732916000	-1.238989000
H	-0.920534000	4.626329000	-2.947119000
H	-0.304837000	3.435570000	-1.774068000
H	-3.602211000	-5.479921000	2.476154000
H	-3.746800000	-3.315917000	-2.078072000
H	-5.390559000	-3.520558000	-1.477302000
H	-6.648399000	0.472537000	-3.739656000
H	0.458344000	0.876735000	1.104024000
H	-0.248983000	1.337425000	-0.915236000
Ti	1.301597000	0.385006000	-0.482730000
P	1.525109000	-1.401489000	-2.307934000
P	2.860829000	2.358819000	0.212765000
N	3.142778000	-0.636519000	0.065579000
C	4.112187000	-0.041572000	0.908111000
C	5.153879000	1.975719000	1.853507000
H	5.179321000	3.062102000	1.945147000
C	4.046967000	-4.565318000	-1.343677000
C	3.440824000	-1.947418000	-0.375752000
C	5.069910000	-0.812483000	1.629315000
C	4.370478000	-2.788162000	0.300628000
C	4.671492000	-4.060763000	-0.196737000
H	5.394247000	-4.674182000	0.343847000
C	4.946645000	-2.315248000	1.611250000
C	2.796266000	-2.474286000	-1.538516000
C	3.096840000	-3.769567000	-1.993971000
H	2.583600000	-4.159540000	-2.872325000
C	6.053781000	-0.186476000	2.401732000
H	6.774544000	-0.810005000	2.933273000
C	4.163898000	1.378066000	1.054262000
C	2.603710000	-1.923270000	-4.970683000
H	3.349123000	-2.626379000	-4.574819000
H	3.027225000	-1.466296000	-5.878070000
H	1.714195000	-2.491378000	-5.273314000
C	6.114362000	1.207616000	2.519841000
C	2.281659000	-0.822599000	-3.944959000
H	1.510354000	-0.153744000	-4.358228000
C	3.527176000	0.025299000	-3.632948000
H	3.272661000	0.836832000	-2.938800000
H	3.926899000	0.472732000	-4.555324000
H	4.317968000	-0.586409000	-3.176561000
C	0.162595000	-2.585698000	-2.841120000
H	0.609562000	-3.273137000	-3.576514000
C	2.367553000	3.613664000	1.546323000
H	3.267050000	4.229102000	1.717137000
C	3.814183000	3.504413000	-0.990160000
H	4.056463000	4.402579000	-0.397930000
C	2.920806000	3.926312000	-2.174107000
H	2.622265000	3.055101000	-2.771013000
H	3.471757000	4.623246000	-2.824274000
H	2.001071000	4.424330000	-1.845446000
C	-0.368527000	-3.412569000	-1.656504000
H	0.423237000	-4.015758000	-1.194960000
H	-1.154927000	-4.096097000	-2.011356000
H	-0.796808000	-2.757886000	-0.889058000
C	-0.971486000	-1.796712000	-3.525374000
H	-1.420203000	-1.083346000	-2.823128000
H	-1.756893000	-2.491062000	-3.859670000
H	-0.621479000	-1.241449000	-4.406554000
C	5.137296000	2.895020000	-1.494047000
H	5.837405000	2.698696000	-0.674195000
H	5.614795000	3.595352000	-2.196241000
H	4.970897000	1.950159000	-2.026347000
C	1.974361000	2.937315000	2.870858000
H	1.100393000	2.292685000	2.729697000
H	1.717083000	3.710345000	3.610473000
H	2.794122000	2.332176000	3.277154000
C	1.236537000	4.529311000	1.039237000
H	1.541107000	5.122613000	0.167261000
H	0.946011000	5.230371000	1.835676000
H	0.354336000	3.936610000	0.767875000
H	4.287466000	-5.559940000	-1.715996000
H	4.275987000	-2.631540000	2.434053000
H	5.917487000	-2.792282000	1.809963000
H	6.886265000	1.682255000	3.123685000
H	0.946116000	1.357913000	-1.957685000
H	-0.204128000	-0.687440000	-0.217902000
N	-1.696933000	2.863046000	2.805392000
N	-1.601500000	2.083339000	1.963632000

F(open-shell singlet)

Ti	1.426525000	0.530183000	-0.553044000
P	1.704321000	-1.322630000	-2.301709000
P	3.009235000	2.406901000	0.451626000
N	3.112212000	-0.608149000	0.214951000
C	4.088768000	-0.077835000	1.093093000
C	5.324658000	1.860650000	1.986925000
H	5.438812000	2.943431000	2.060166000
C	3.763510000	-4.670614000	-0.984403000
C	3.315936000	-1.966164000	-0.151396000
C	4.948542000	-0.906464000	1.874178000
C	4.108558000	-2.860292000	0.621806000
C	4.336137000	-4.172765000	0.192009000
H	4.959063000	-4.820887000	0.811127000
C	4.638206000	-2.379685000	1.948676000
C	2.730242000	-2.485894000	-1.344797000
C	2.950841000	-3.818244000	-1.738034000
H	2.479164000	-4.190032000	-2.647477000
C	6.001693000	-0.355455000	2.610404000
H	6.649872000	-1.029993000	3.172739000
C	4.270699000	1.332099000	1.218852000
C	2.822343000	-1.982231000	-4.924946000
H	3.235823000	-2.922753000	-4.534702000
H	3.488042000	-1.640136000	-5.732208000
H	1.842364000	-2.190055000	-5.373213000
C	6.219153000	1.028171000	2.664081000
C	2.757997000	-0.902490000	-3.828850000
H	2.280042000	-0.003531000	-4.246903000
C	4.179548000	-0.525165000	-3.366030000
H	4.159538000	0.191134000	-2.536330000
H	4.739230000	-0.076063000	-4.199975000
H	4.724184000	-1.415990000	-3.025510000
C	0.285548000	-2.339938000	-3.011771000
H	0.732722000	-3.063951000	-3.710363000
C	2.428937000	3.476123000	1.912595000
H	3.249292000	4.185304000	2.114864000
C	4.080806000	3.613025000	-0.549052000
H	4.821571000	3.991562000	0.174492000
C	3.314787000	4.815306000	-1.134966000
H	2.471572000	4.492732000	-1.758744000
H	3.995956000	5.400354000	-1.771186000

H	2.938598000	5.487770000	-0.354758000
C	-0.481088000	-3.117858000	-1.928629000
H	0.170390000	-3.824096000	-1.399881000
H	-1.297286000	-3.688571000	-2.397108000
H	-0.917465000	-2.435480000	-1.190395000
C	-0.657759000	-1.407895000	-3.800673000
H	-1.118630000	-0.672592000	-3.127429000
H	-1.463094000	-1.996712000	-4.264851000
H	-0.137519000	-0.861222000	-4.599776000
C	4.835243000	2.857396000	-1.659201000
H	5.379112000	1.990433000	-1.263428000
H	5.564818000	3.532344000	-2.131368000
H	4.143490000	2.514278000	-2.438166000
C	2.196279000	2.619509000	3.173721000
H	1.453170000	1.833100000	2.980229000
H	1.809077000	3.257241000	3.982937000
H	3.116802000	2.138059000	3.521378000
C	1.148492000	4.266462000	1.574222000
H	1.271401000	4.933637000	0.714017000
H	0.859386000	4.882508000	2.439625000
H	0.326443000	3.577605000	1.345892000
H	3.937300000	-5.698654000	-1.298573000
H	3.871981000	-2.548381000	2.730862000
H	5.523041000	-2.956541000	2.254778000
H	7.042853000	1.443233000	3.242669000
H	-0.006612000	1.623862000	-0.022090000
H	-0.588198000	1.498555000	1.981033000
Ti	-1.430631000	0.458036000	0.439032000
P	-1.630789000	-1.309762000	2.288194000
P	-3.167574000	2.349562000	-0.203473000
N	-3.176327000	-0.646983000	-0.146985000
C	-4.223574000	-0.108490000	-0.929921000
C	-5.535156000	1.831317000	-1.692887000
H	-5.679777000	2.912562000	-1.717989000
C	-3.804653000	-4.664792000	1.149148000
C	-3.369537000	-1.993058000	0.248271000
C	-5.104259000	-0.934912000	-1.687569000
C	-4.200648000	-2.888193000	-0.479099000
C	-4.421597000	-4.189873000	-0.015630000
H	-5.072091000	-4.847783000	-0.594663000
C	-4.771884000	-2.404010000	-1.789567000
C	-2.738532000	-2.483287000	1.429911000
C	-2.954773000	-3.807122000	1.855736000
H	-2.453037000	-4.169891000	2.752564000
C	-6.195091000	-0.381675000	-2.364207000
H	-6.857686000	-1.048803000	-2.918424000
C	-4.447615000	1.299326000	-0.974325000
C	-2.805365000	-1.889536000	4.905034000
H	-3.376517000	-2.726734000	4.480809000
H	-3.387075000	-1.483919000	5.747062000
H	-1.864236000	-2.280045000	5.313154000
C	-6.431970000	1.000833000	-2.370260000
C	-2.581975000	-0.787722000	3.853583000
H	-1.955312000	0.004338000	4.296592000
C	-3.925379000	-0.161095000	3.434247000
H	-3.778723000	0.626644000	2.683408000
H	-4.431323000	0.276031000	4.308377000
H	-4.588314000	-0.918871000	2.995008000
C	-0.238156000	-2.375865000	2.979981000
H	-0.692460000	-3.094800000	3.679259000
C	-2.681345000	3.446244000	-1.669603000
H	-3.599284000	3.986014000	-1.957053000
C	-4.066552000	3.606284000	0.917718000
H	-4.286707000	4.467855000	0.266178000
C	-3.138347000	4.078879000	2.055979000
H	-2.948223000	3.259275000	2.763307000
H	-3.615939000	4.899143000	2.612754000
H	-2.168501000	4.436519000	1.688054000
C	0.475757000	-3.157553000	1.864041000
H	-0.207523000	-3.847686000	1.354571000
H	1.301607000	-3.745319000	2.292138000
H	0.891962000	-2.473762000	1.115660000
C	0.753941000	-1.490099000	3.760432000
H	1.230492000	-0.764171000	3.087464000
H	1.546675000	-2.113808000	4.199962000
H	0.270970000	-0.939179000	4.580158000
C	-5.395005000	3.081285000	1.494949000
H	-6.106634000	2.800907000	0.710946000
H	-5.854399000	3.864753000	2.116691000
H	-5.234071000	2.201592000	2.130910000
C	-2.226546000	2.573650000	-2.854153000
H	-1.367510000	1.951758000	-2.570659000
H	-1.912628000	3.214889000	-3.690863000
H	-3.033238000	1.918335000	-3.203789000
C	-1.597839000	4.470260000	-1.286209000
H	-1.925214000	5.143110000	-0.481808000
H	-1.352891000	5.091892000	-2.160345000
H	-0.682837000	3.957427000	-0.964758000
H	-3.974440000	-5.684388000	1.492001000
H	-4.019122000	-2.548473000	-2.589430000
H	-5.653623000	-2.992141000	-2.081936000
H	-7.280762000	1.418311000	-2.909592000
H	-1.339359000	1.661229000	2.097871000
H	-0.002624000	-0.602392000	-0.166865000
N	1.311745000	2.330012000	-3.149263000
N	1.293031000	1.679821000	-2.200260000

F(triplet)

Ti	1.411926000	0.518750000	-0.537243000
P	1.702985000	-1.329733000	-2.288989000
P	2.952308000	2.422249000	0.446147000
N	3.125166000	-0.581390000	0.205227000
C	4.096857000	-0.032515000	1.079049000
C	5.293391000	1.932392000	1.966461000
H	5.384850000	3.017372000	2.038226000
C	3.858929000	-4.629268000	-1.002704000
C	3.355956000	-1.936118000	-0.163654000
C	4.979170000	-0.842787000	1.853090000
C	4.174189000	-2.812427000	0.602966000
C	4.428426000	-4.119173000	0.169798000
H	5.070971000	-4.753094000	0.783549000
C	4.703380000	-2.322739000	1.926692000
C	2.770548000	-2.469841000	-1.350754000
C	3.019537000	-3.795661000	-1.748182000
H	2.547974000	-4.177236000	-2.653675000
C	6.023586000	-0.268640000	2.584697000
H	6.689949000	-0.928821000	3.142784000
C	4.247703000	1.380343000	1.204213000
C	2.764931000	-1.953412000	-4.943814000
H	3.193543000	-2.895750000	-4.574671000
H	3.409657000	-1.597499000	-5.762066000
H	1.776290000	-2.162552000	-5.371936000
C	6.209860000	1.119314000	2.638295000
C	2.719536000	-0.885847000	-3.834842000
H	2.226709000	0.014414000	-4.231471000
C	4.149284000	-0.505130000	-3.400848000
H	4.144214000	0.198440000	-2.560183000
H	4.684593000	-0.039080000	-4.241443000
H	4.708692000	-1.396844000	-3.087631000
C	0.292288000	-2.376717000	-2.972239000
H	0.739724000	-3.086521000	-3.685043000
C	2.382257000	3.485798000	1.915090000
H	3.212020000	4.181154000	2.126334000
C	3.988314000	3.636725000	-0.583356000
H	4.725092000	4.046366000	0.127372000
C	3.192317000	4.807706000	-1.192736000
H	2.349117000	4.450991000	-1.797328000
H	3.855001000	5.387154000	-1.853234000

H	2.812357000	5.495365000	-0.428008000
C	-0.431546000	-3.176955000	-1.876079000
H	0.246579000	-3.873387000	-1.368109000
H	-1.247790000	-3.760791000	-2.328021000
H	-0.864043000	-2.507429000	-1.123758000
C	-0.689964000	-1.461108000	-3.731993000
H	-1.151474000	-0.742801000	-3.040955000
H	-1.491656000	-2.064995000	-4.183056000
H	-0.200840000	-0.895184000	-4.537239000
C	4.751081000	2.875603000	-1.684350000
H	5.315891000	2.027503000	-1.277194000
H	5.462889000	3.556861000	-2.174343000
H	4.060078000	2.504871000	-2.451170000
C	2.139248000	2.614684000	3.164572000
H	1.379679000	1.846715000	2.962594000
H	1.770262000	3.247509000	3.986154000
H	3.052350000	2.110132000	3.499055000
C	1.113201000	4.299785000	1.591451000
H	1.251076000	4.995955000	0.757245000
H	0.820573000	4.887421000	2.475165000
H	0.286052000	3.628428000	1.330888000
H	4.054437000	-5.652659000	-1.319304000
H	3.947879000	-2.511071000	2.714892000
H	5.603746000	-2.879833000	2.224021000
H	7.027778000	1.552294000	3.211984000
H	0.017291000	1.618649000	0.068689000
H	-0.670800000	1.697973000	1.873290000
Ti	-1.427028000	0.452471000	0.443297000
P	-1.594459000	-1.306417000	2.301027000
P	-3.177135000	2.334835000	-0.225066000
N	-3.168155000	-0.662567000	-0.129045000
C	-4.222335000	-0.139266000	-0.913847000
C	-5.549593000	1.783960000	-1.692254000
H	-5.699926000	2.864072000	-1.729503000
C	-3.732618000	-4.687894000	1.177413000
C	-3.341009000	-2.010552000	0.269812000
C	-5.100420000	-0.978846000	-1.659770000
C	-4.167055000	-2.917894000	-0.448323000
C	-4.366601000	-4.221879000	0.018411000
H	-5.014016000	-4.888536000	-0.554000000
C	-4.757396000	-2.445852000	-1.754555000
C	-2.693407000	-2.491804000	1.446741000
C	-2.887947000	-3.818198000	1.875266000
H	-2.373517000	-4.173381000	2.767868000
C	-6.198720000	-0.439866000	-2.336041000
H	-6.859045000	-1.117165000	-2.880522000
C	-4.454628000	1.266676000	-0.974349000
C	-2.773859000	-1.902733000	4.911161000
H	-3.342773000	-2.738274000	4.480818000
H	-3.357502000	-1.503015000	5.754596000
H	-1.832622000	-2.293879000	5.318345000
C	-6.445501000	0.940651000	-2.354714000
C	-2.550724000	-0.794256000	3.866712000
H	-1.926471000	-0.003658000	4.316068000
C	-3.895063000	-0.168349000	3.448962000
H	-3.750238000	0.628825000	2.707572000
H	-4.405819000	0.257338000	4.325870000
H	-4.553403000	-0.923726000	2.998947000
C	-0.189491000	-2.355722000	2.993771000
H	-0.636676000	-3.080964000	3.691098000
C	-2.706505000	3.422289000	-1.702121000
H	-3.625508000	3.964972000	-1.980727000
C	-4.078351000	3.591489000	0.894237000
H	-4.310170000	4.446775000	0.238469000
C	-3.147270000	4.079752000	2.023690000
H	-2.946472000	3.267475000	2.735994000
H	-3.628365000	4.900550000	2.576526000
H	-2.182548000	4.442336000	1.647592000
C	0.536078000	-3.126711000	1.878195000
H	-0.137224000	-3.824205000	1.365651000
H	1.368093000	-3.704863000	2.307352000
H	0.946234000	-2.436328000	1.132387000
C	0.790192000	-1.458925000	3.777210000
H	1.256906000	-0.724281000	3.106920000
H	1.591114000	-2.073716000	4.214340000
H	0.299883000	-0.917720000	4.598986000
C	-5.398510000	3.058922000	1.483513000
H	-6.113748000	2.769626000	0.706091000
H	-5.859182000	3.841680000	2.105179000
H	-5.226298000	2.183234000	2.122165000
C	-2.268796000	2.544192000	-2.889195000
H	-1.411028000	1.916770000	-2.614854000
H	-1.958459000	3.182311000	-3.729434000
H	-3.083681000	1.894435000	-3.229983000
C	-1.614781000	4.442952000	-1.332425000
H	-1.932256000	5.120149000	-0.527649000
H	-1.374788000	5.059990000	-2.211040000
H	-0.698981000	3.927588000	-1.017273000
H	-3.885643000	-5.709300000	1.522675000
H	-4.013364000	-2.590109000	-2.562519000
H	-5.637801000	-3.042904000	-2.032604000
H	-7.300064000	1.346780000	-2.893551000
H	-1.348738000	1.519765000	2.203600000
H	-0.023029000	-0.604212000	-0.179178000
N	1.236323000	2.274185000	-3.149296000
N	1.228688000	1.638022000	-2.186113000

F(quintet)

Ti	1.422080000	0.546276000	-0.565215000
P	1.730103000	-1.291092000	-2.329548000
P	3.018230000	2.375221000	0.488672000
N	3.077483000	-0.632889000	0.232984000
C	4.051175000	-0.127178000	1.123834000
C	5.316098000	1.783379000	2.035709000
H	5.451085000	2.863325000	2.114754000
C	3.669336000	-4.696699000	-0.985029000
C	3.261232000	-1.988894000	-0.140382000
C	4.885268000	-0.975824000	1.912135000
C	4.021255000	-2.905294000	0.641094000
C	4.229366000	-4.218739000	0.206322000
H	4.826590000	-4.884148000	0.832426000
C	4.538332000	-2.441304000	1.978973000
C	2.692598000	-2.487197000	-1.351194000
C	2.892947000	-3.821472000	-1.750027000
H	2.434159000	-4.176410000	-2.672736000
C	5.942383000	-0.448728000	2.659039000
H	6.570943000	-1.137268000	3.226697000
C	4.258463000	1.278340000	1.256159000
C	2.928552000	-1.962105000	-4.911580000
H	3.317964000	-2.906509000	-4.506344000
H	3.625044000	-1.628305000	-5.695950000
H	1.962120000	-2.159708000	-5.392864000
C	6.187557000	0.930784000	2.717495000
C	2.838365000	-0.880928000	-3.818857000
H	2.384221000	0.023108000	-4.252590000
C	4.246169000	-0.517931000	-3.305535000
H	4.202819000	0.202750000	-2.480429000
H	4.841486000	-0.079559000	-4.120268000
H	4.767252000	-1.413397000	-2.941092000
C	0.308559000	-2.265128000	-3.092760000
H	0.759885000	-3.001759000	-3.775371000
C	2.429292000	3.423786000	1.964846000
H	3.250288000	4.128659000	2.179302000
C	4.110517000	3.600676000	-0.466438000
H	4.835464000	3.966094000	0.279558000
C	3.355535000	4.814774000	-1.042537000
H	2.525596000	4.505675000	-1.690376000
H	4.048750000	5.414356000	-1.651685000

H	2.962173000	5.469680000	-0.255789000
C	-0.515748000	-3.020691000	-2.036345000
H	0.098735000	-3.739490000	-1.480907000
H	-1.327379000	-3.574098000	-2.532749000
H	-0.961969000	-2.325683000	-1.315956000
C	-0.580799000	-1.309706000	-3.915569000
H	-1.052510000	-0.564458000	-3.260939000
H	-1.380432000	-1.878611000	-4.413159000
H	-0.016383000	-0.774199000	-4.691802000
C	4.890094000	2.868170000	-1.574613000
H	5.429577000	1.996737000	-1.182724000
H	5.626088000	3.554445000	-2.019879000
H	4.216336000	2.535122000	-2.373320000
C	2.191471000	2.551834000	3.214044000
H	1.449130000	1.767717000	3.008054000
H	1.800514000	3.179464000	4.029429000
H	3.110262000	2.065748000	3.559613000
C	1.151167000	4.219980000	1.634086000
H	1.276212000	4.896548000	0.781494000
H	0.860971000	4.826765000	2.505772000
H	0.329011000	3.534025000	1.397075000
H	3.826319000	-5.726520000	-1.302178000
H	3.753569000	-2.591874000	2.746433000
H	5.402901000	-3.040424000	2.299786000
H	7.014371000	1.327528000	3.304481000
H	-0.028024000	1.635680000	-0.037772000
H	-0.640837000	1.401780000	2.119550000
Ti	-1.417882000	0.445198000	0.474840000
P	-1.702332000	-1.341633000	2.294184000
P	-3.116414000	2.368250000	-0.175756000
N	-3.153674000	-0.624901000	-0.182956000
C	-4.176116000	-0.061856000	-0.981633000
C	-5.451359000	1.904391000	-1.734770000
H	-5.587221000	2.986973000	-1.740165000
C	-3.875228000	-4.652486000	1.034958000
C	-3.377301000	-1.973799000	0.188770000
C	-5.043688000	-0.865155000	-1.777464000
C	-4.195825000	-2.847160000	-0.578494000
C	-4.447857000	-4.152394000	-0.141955000
H	-5.087674000	-4.793065000	-0.751356000
C	-4.721487000	-2.335008000	-1.897378000
C	-2.792434000	-2.489356000	1.382736000
C	-3.038836000	-3.816297000	1.781915000
H	-2.570788000	-4.198199000	2.688921000
C	-6.112167000	-0.288538000	-2.470067000
H	-6.766076000	-0.937854000	-3.054824000
C	-4.387054000	1.347687000	-1.000043000
C	-2.953323000	-1.963475000	4.865608000
H	-3.527695000	-2.781031000	4.408842000
H	-3.548251000	-1.567185000	5.702780000
H	-2.028744000	-2.379031000	5.286686000
C	-6.336801000	1.095955000	-2.452501000
C	-2.686568000	-0.842157000	3.845430000
H	-2.060977000	-0.069384000	4.322683000
C	-4.008460000	-0.186520000	3.402906000
H	-3.829161000	0.612410000	2.671076000
H	-4.531103000	0.242459000	4.271139000
H	-4.670974000	-0.925358000	2.931859000
C	-0.329251000	-2.426898000	2.994837000
H	-0.802744000	-3.152531000	3.674267000
C	-2.589568000	3.486974000	-1.613922000
H	-3.500537000	4.035440000	-1.907157000
C	-4.034890000	3.620441000	0.936857000
H	-4.231213000	4.491604000	0.290491000
C	-3.133667000	4.072433000	2.104763000
H	-2.970536000	3.243860000	2.808720000
H	-3.618967000	4.890721000	2.657739000
H	-2.151075000	4.425977000	1.767648000
C	0.400537000	-3.198436000	1.881634000
H	-0.279103000	-3.873247000	1.347174000
H	1.209796000	-3.802175000	2.319048000
H	0.840039000	-2.508505000	1.152655000
C	0.653285000	-1.560426000	3.808581000
H	1.149273000	-0.827605000	3.157559000
H	1.432449000	-2.196761000	4.254091000
H	0.157867000	-1.018940000	4.627191000
C	-5.381804000	3.099628000	1.473660000
H	-6.075275000	2.833971000	0.668557000
H	-5.851123000	3.879379000	2.092687000
H	-5.244082000	2.211387000	2.103178000
C	-2.117387000	2.636544000	-2.807075000
H	-1.261535000	2.011349000	-2.521897000
H	-1.792833000	3.293843000	-3.627152000
H	-2.917865000	1.986766000	-3.180532000
C	-1.509190000	4.499453000	-1.195047000
H	-1.844787000	5.158006000	-0.382282000
H	-1.250004000	5.136983000	-2.053588000
H	-0.600865000	3.976383000	-0.872030000
H	-4.068275000	-5.674963000	1.356160000
H	-3.945533000	-2.471871000	-2.675928000
H	-5.598941000	-2.909493000	-2.227138000
H	-7.168208000	1.532234000	-3.003909000
H	-1.350406000	1.711520000	2.096187000
H	0.033512000	-0.633937000	-0.076652000
N	1.439830000	2.373514000	-3.150064000
N	1.408462000	1.719812000	-2.203729000

TS_{FG}(open-shell singlet)

Ti	1.426992000	0.501155000	-0.489204000
P	1.723635000	-1.348596000	-2.250072000
P	3.030583000	2.423480000	0.380799000
N	3.150133000	-0.591756000	0.231562000
C	4.143267000	-0.030723000	1.073472000
C	5.385034000	1.936459000	1.886072000
H	5.495062000	3.021348000	1.927601000
C	3.872647000	-4.647320000	-0.940842000
C	3.374541000	-1.949948000	-0.123930000
C	5.023906000	-0.835348000	1.855094000
C	4.191694000	-2.819559000	0.650683000
C	4.443120000	-4.130283000	0.228576000
H	5.084562000	-4.761126000	0.846598000
C	4.724512000	-2.309085000	1.965380000
C	2.787793000	-2.489356000	-1.306831000
C	3.035206000	-3.818423000	-1.694182000
H	2.566285000	-4.205898000	-2.598658000
C	6.088883000	-0.259468000	2.554653000
H	6.753846000	-0.914902000	3.119954000
C	4.317539000	1.382648000	1.155624000
C	2.749971000	-1.957698000	-4.925149000
H	3.148454000	-2.920692000	-4.575648000
H	3.402733000	-1.608401000	-5.739901000
H	1.753052000	-2.126302000	-5.351986000
C	6.297886000	1.126431000	2.566558000
C	2.744935000	-0.910580000	-3.795782000
H	2.278521000	0.012380000	-4.172410000
C	4.189483000	-0.585330000	-3.364656000
H	4.214234000	0.089130000	-2.500872000
H	4.730056000	-0.107110000	-4.195032000
H	4.724994000	-1.503215000	-3.087654000
C	0.315234000	-2.400676000	-2.929139000
H	0.764104000	-3.103253000	-3.648144000
C	2.483738000	3.554991000	1.806925000
H	3.295555000	4.289567000	1.942763000
C	4.072176000	3.596331000	-0.689678000
H	4.840069000	3.988574000	-0.002408000
C	3.292029000	4.789201000	-1.276098000
H	2.431588000	4.456830000	-1.870485000
H	3.956582000	5.361128000	-1.941361000

H	2.938844000	5.476287000	-0.497670000
C	-0.398029000	-3.213980000	-1.835043000
H	0.287327000	-3.908654000	-1.334419000
H	-1.211302000	-3.801052000	-2.288309000
H	-0.832225000	-2.553292000	-1.076123000
C	-0.677483000	-1.489130000	-3.679864000
H	-1.145326000	-0.781835000	-2.981824000
H	-1.473933000	-2.096810000	-4.135184000
H	-0.195299000	-0.910746000	-4.480498000
C	4.781937000	2.808960000	-1.806041000
H	5.348384000	1.959372000	-1.404292000
H	5.486197000	3.470581000	-2.332660000
H	4.058526000	2.434807000	-2.540797000
C	2.309889000	2.758375000	3.115216000
H	1.584539000	1.945285000	2.978966000
H	1.924055000	3.424286000	3.902075000
H	3.253000000	2.321687000	3.461504000
C	1.175082000	4.301011000	1.473410000
H	1.246840000	4.905626000	0.562274000
H	0.915767000	4.973916000	2.305364000
H	0.357823000	3.582790000	1.336453000
H	4.067314000	-5.673123000	-1.250161000
H	3.962713000	-2.465091000	2.754535000
H	5.614798000	-2.873138000	2.279061000
H	7.130895000	1.561388000	3.116599000
H	0.123915000	1.522833000	0.399260000
H	-0.761204000	1.827712000	2.883411000
Ti	-1.463262000	0.443219000	0.373175000
P	-1.620148000	-1.203540000	2.335531000
P	-3.283850000	2.310224000	-0.247615000
N	-3.176673000	-0.692644000	-0.142247000
C	-4.244577000	-0.209801000	-0.932063000
C	-5.609619000	1.665751000	-1.752731000
H	-5.789087000	2.740595000	-1.809216000
C	-3.631322000	-4.688451000	1.271304000
C	-3.320897000	-2.030300000	0.299019000
C	-5.097983000	-1.086925000	-1.662185000
C	-4.119239000	-2.975990000	-0.398172000
C	-4.278636000	-4.273923000	0.100036000
H	-4.903847000	-4.975647000	-0.454797000
C	-4.722053000	-2.549087000	-1.715471000
C	-2.666946000	-2.452712000	1.493763000
C	-2.819434000	-3.774794000	1.952570000
H	-2.302108000	-4.091495000	2.857695000
C	-6.201305000	-0.586951000	-2.359519000
H	-6.843370000	-1.288859000	-2.894488000
C	-4.511921000	1.188842000	-1.010218000
C	-2.953408000	-1.832619000	4.861528000
H	-3.551942000	-2.616497000	4.378309000
H	-3.543619000	-1.430232000	5.699174000
H	-2.052767000	-2.294099000	5.286986000
C	-6.475827000	0.787981000	-2.409843000
C	-2.625671000	-0.700152000	3.872092000
H	-1.988774000	0.040539000	4.381136000
C	-3.912562000	0.007991000	3.410694000
H	-3.683809000	0.835878000	2.726410000
H	-4.459411000	0.410659000	4.276815000
H	-4.574620000	-0.689361000	2.879299000
C	-0.198355000	-2.195096000	3.082269000
H	-0.636296000	-2.905925000	3.799919000
C	-2.780835000	3.348394000	-1.751057000
H	-3.696088000	3.863852000	-2.087238000
C	-4.262370000	3.587005000	0.779095000
H	-4.524641000	4.386596000	0.066906000
C	-3.376100000	4.190290000	1.889038000
H	-3.164661000	3.439438000	2.661928000
H	-3.900858000	5.029244000	2.370190000
H	-2.415574000	4.561558000	1.510928000
C	0.561001000	-2.987237000	2.004292000
H	-0.088834000	-3.713966000	1.502260000
H	1.396362000	-3.534638000	2.466099000
H	0.970088000	-2.313222000	1.242860000
C	0.750519000	-1.248910000	3.845176000
H	1.204545000	-0.524107000	3.155782000
H	1.563278000	-1.828192000	4.308144000
H	0.239279000	-0.694644000	4.644830000
C	-5.564225000	3.026157000	1.383024000
H	-6.251250000	2.652965000	0.615955000
H	-6.073250000	3.822637000	1.946751000
H	-5.359118000	2.202898000	2.078932000
C	-2.291869000	2.421200000	-2.879651000
H	-1.449189000	1.802092000	-2.542313000
H	-1.937077000	3.020465000	-3.730499000
H	-3.092052000	1.758368000	-3.229545000
C	-1.716018000	4.400791000	-1.390716000
H	-2.077956000	5.118282000	-0.641976000
H	-1.440729000	4.969825000	-2.291027000
H	-0.809565000	3.918421000	-1.003629000
H	-3.752572000	-5.705105000	1.642365000
H	-3.975992000	-2.698534000	-2.520453000
H	-5.589421000	-3.172334000	-1.976428000
H	-7.334001000	1.163674000	-2.964854000
H	-1.253696000	2.254798000	3.238371000
H	-0.034161000	-0.627003000	-0.212230000
N	1.157327000	2.300023000	-3.064116000
N	1.178935000	1.651049000	-2.110417000

TS_{FG}(triplet)

Ti	1.408519000	0.482597000	-0.474256000
P	1.728211000	-1.374229000	-2.226232000
P	2.954657000	2.445547000	0.368314000
N	3.167208000	-0.558201000	0.223181000
C	4.155788000	0.033497000	1.050879000
C	5.352289000	2.039498000	1.833642000
H	5.432916000	3.127210000	1.866561000
C	3.975653000	-4.608401000	-0.919311000
C	3.421904000	-1.915202000	-0.122750000
C	5.067260000	-0.741576000	1.825956000
C	4.269553000	-2.756581000	0.649898000
C	4.547251000	-4.065434000	0.237481000
H	5.211638000	-4.673884000	0.853721000
C	4.808110000	-2.221490000	1.952394000
C	2.833692000	-2.481794000	-1.292151000
C	3.109067000	-3.807625000	-1.670403000
H	2.638260000	-4.214922000	-2.565170000
C	6.125493000	-0.131722000	2.507386000
H	6.815274000	-0.764572000	3.068653000
C	4.290931000	1.451094000	1.122072000
C	2.732689000	-1.965594000	-4.910499000
H	3.158367000	-2.917858000	-4.563502000
H	3.365932000	-1.603959000	-5.735199000
H	1.734248000	-2.158780000	-5.323034000
C	6.296725000	1.259199000	2.506264000
C	2.719203000	-0.914488000	-3.784886000
H	2.226664000	-0.003565000	-4.156871000
C	4.161796000	-0.555758000	-3.374359000
H	4.183055000	0.122449000	-2.513524000
H	4.679608000	-0.068543000	-4.213924000
H	4.721792000	-1.460333000	-3.101904000
C	0.336876000	-2.461298000	-2.883169000
H	0.791746000	-3.159665000	-3.602505000
C	2.409984000	3.564673000	1.805141000
H	3.212220000	4.311167000	1.932578000
C	3.937342000	3.641643000	-0.732321000
H	4.703401000	4.067905000	-0.063424000
C	3.107821000	4.799646000	-1.321143000
H	2.247872000	4.429856000	-1.893538000
H	3.740750000	5.381804000	-2.008089000

H	2.747745000	5.487728000	-0.546857000
C	-0.344992000	-3.279490000	-1.772914000
H	0.359584000	-3.960716000	-1.280362000
H	-1.157410000	-3.881251000	-2.207916000
H	-0.776403000	-2.620360000	-1.010937000
C	-0.683764000	-1.575375000	-3.627036000
H	-1.156223000	-0.872711000	-2.927395000
H	-1.473029000	-2.202828000	-4.067925000
H	-0.223592000	-0.992930000	-4.437494000
C	4.652742000	2.864720000	-1.852608000
H	5.254952000	2.039384000	-1.452257000
H	5.324587000	3.543259000	-2.399768000
H	3.928122000	2.458873000	-2.569088000
C	2.269504000	2.757107000	3.110804000
H	1.557652000	1.931570000	2.978000000
H	1.883427000	3.410495000	3.907990000
H	3.225329000	2.335056000	3.440144000
C	1.085247000	4.292843000	1.497747000
H	1.138899000	4.918973000	0.600244000
H	0.820020000	4.942100000	2.346455000
H	0.279765000	3.563195000	1.350667000
H	4.191408000	-5.632410000	-1.220490000
H	4.062666000	-2.390846000	2.754413000
H	5.717357000	-2.759717000	2.256968000
H	7.125627000	1.720623000	3.040771000
H	0.144059000	1.479919000	0.482275000
H	-0.759295000	1.880513000	2.931226000
Ti	-1.454323000	0.435582000	0.392990000
P	-1.592468000	-1.226752000	2.341903000
P	-3.271487000	2.301028000	-0.260847000
N	-3.167681000	-0.700000000	-0.128669000
C	-4.246469000	-0.220847000	-0.907218000
C	-5.631222000	1.649580000	-1.707146000
H	-5.813830000	2.723945000	-1.762180000
C	-3.555774000	-4.722395000	1.236530000
C	-3.291908000	-2.044998000	0.297719000
C	-5.103518000	-1.099907000	-1.630558000
C	-4.086953000	-2.992193000	-0.401580000
C	-4.222737000	-4.299215000	0.079699000
H	-4.845859000	-5.000714000	-0.477719000
C	-4.715704000	-2.557776000	-1.703808000
C	-2.621655000	-2.476144000	1.481072000
C	-2.750316000	-3.806786000	1.922273000
H	-2.220498000	-4.127908000	2.818519000
C	-6.220657000	-0.604307000	-2.309030000
H	-6.865409000	-1.308451000	-2.837774000
C	-4.518891000	1.176608000	-0.984640000
C	-2.960457000	-1.893260000	4.836366000
H	-3.550888000	-2.669454000	4.331296000
H	-3.562825000	-1.505148000	5.672029000
H	-2.065499000	-2.361129000	5.266807000
C	-6.505269000	0.768703000	-2.349649000
C	-2.619128000	-0.744303000	3.870766000
H	-1.989285000	-0.012551000	4.400997000
C	-3.899558000	-0.028734000	3.402401000
H	-3.662401000	0.814918000	2.740356000
H	-4.461826000	0.354335000	4.267519000
H	-4.551208000	-0.715146000	2.844781000
C	-0.165607000	-2.203836000	3.096811000
H	-0.601474000	-2.927673000	3.802646000
C	-2.790244000	3.316495000	-1.787076000
H	-3.706801000	3.843672000	-2.101144000
C	-4.225825000	3.594767000	0.766952000
H	-4.506307000	4.380338000	0.046160000
C	-3.315851000	4.220655000	1.844574000
H	-3.086139000	3.486164000	2.627694000
H	-3.831187000	5.068654000	2.319997000
H	-2.364472000	4.585017000	1.438367000
C	0.619621000	-2.973426000	2.021207000
H	-0.011793000	-3.704556000	1.502557000
H	1.457175000	-3.512490000	2.488753000
H	1.029267000	-2.285083000	1.272782000
C	0.759714000	-1.250327000	3.879468000
H	1.207415000	-0.509902000	3.202693000
H	1.577746000	-1.821716000	4.342799000
H	0.232080000	-0.714436000	4.680863000
C	-5.512359000	3.044400000	1.412092000
H	-6.214574000	2.650299000	0.669656000
H	-6.011858000	3.852749000	1.967338000
H	-5.289099000	2.239317000	2.123567000
C	-2.348060000	2.374648000	-2.922926000
H	-1.508876000	1.741328000	-2.605683000
H	-2.005648000	2.964879000	-3.784939000
H	-3.170225000	1.726515000	-3.248526000
C	-1.700738000	4.355186000	-1.462073000
H	-2.035235000	5.087355000	-0.714776000
H	-1.435854000	4.908580000	-2.375047000
H	-0.794039000	3.862968000	-1.088567000
H	-3.658755000	-5.745833000	1.594121000
H	-3.982834000	-2.692807000	-2.523272000
H	-5.581836000	-3.186492000	-1.955641000
H	-7.374591000	1.140897000	-2.889402000
H	-1.309141000	2.164170000	3.340523000
H	-0.053452000	-0.635061000	-0.209233000
N	1.070226000	2.213996000	-3.077434000
N	1.103595000	1.589390000	-2.103887000

TS_{FG}(quintet)

Ti	1.442315000	0.519749000	-0.545342000
P	1.772431000	-1.362700000	-2.263135000
P	3.029236000	2.413392000	0.392982000
N	3.119720000	-0.599846000	0.262303000
C	4.105508000	-0.045314000	1.112803000
C	5.372012000	1.911912000	1.911405000
H	5.500674000	2.995080000	1.939446000
C	3.775706000	-4.691930000	-0.816932000
C	3.323670000	-1.966472000	-0.064676000
C	4.957198000	-0.852714000	1.923915000
C	4.100503000	-2.840936000	0.746497000
C	4.329206000	-4.165298000	0.356704000
H	4.938826000	-4.799103000	1.003244000
C	4.618568000	-2.315501000	2.061174000
C	2.760978000	-2.513587000	-1.255969000
C	2.983812000	-3.856461000	-1.610560000
H	2.531168000	-4.249595000	-2.520775000
C	6.024571000	-0.285893000	2.626256000
H	6.667811000	-0.943486000	3.213763000
C	4.303388000	1.365722000	1.176168000
C	2.956939000	-2.075519000	-4.841219000
H	3.353440000	-3.010230000	-4.420481000
H	3.647432000	-1.753116000	-5.635618000
H	1.988934000	-2.287119000	-5.313311000
C	6.261737000	1.096076000	2.614787000
C	2.867056000	-0.974294000	-3.768626000
H	2.403055000	-0.081896000	-4.215884000
C	4.276080000	-0.591745000	-3.272871000
H	4.233649000	0.139774000	-2.457298000
H	4.860108000	-0.159236000	-4.098825000
H	4.808352000	-1.477573000	-2.901175000
C	0.365886000	-2.385021000	-2.989076000
H	0.826524000	-3.122872000	-3.664074000
C	2.453764000	3.503561000	1.843633000
H	3.264920000	4.232142000	2.012035000
C	4.078102000	3.624122000	-0.627047000
H	4.813402000	4.026730000	0.089191000
C	3.286479000	4.805593000	-1.221662000
H	2.449358000	4.460619000	-1.841513000
H	3.954093000	5.400491000	-1.863204000

H	2.896711000	5.475215000	-0.445557000
C	-0.427787000	-3.141719000	-1.910065000
H	0.209649000	-3.838772000	-1.352686000
H	-1.233597000	-3.720074000	-2.387050000
H	-0.879095000	-2.445904000	-1.193851000
C	-0.554521000	-1.464686000	-3.817860000
H	-1.029666000	-0.714490000	-3.171264000
H	-1.350826000	-2.058740000	-4.290880000
H	-0.012474000	-0.934922000	-4.613804000
C	4.845000000	2.871130000	-1.729994000
H	5.414153000	2.026048000	-1.322619000
H	5.553770000	3.557169000	-2.217897000
H	4.158672000	2.495583000	-2.498645000
C	2.263256000	2.667443000	3.124428000
H	1.536052000	1.862054000	2.954430000
H	1.869765000	3.309712000	3.926990000
H	3.200758000	2.216990000	3.467847000
C	1.149569000	4.260824000	1.522158000
H	1.225029000	4.885730000	0.625227000
H	0.889129000	4.915514000	2.368244000
H	0.330368000	3.548361000	1.366984000
H	3.950060000	-5.728981000	-1.099642000
H	3.836743000	-2.433792000	2.837235000
H	5.487343000	-2.894775000	2.405829000
H	7.096965000	1.524292000	3.166753000
H	0.063437000	1.612698000	0.158150000
H	-0.914876000	1.746304000	3.215304000
Ti	-1.449827000	0.449891000	0.402275000
P	-1.727261000	-1.205946000	2.356797000
P	-3.244755000	2.325705000	-0.230159000
N	-3.141576000	-0.672387000	-0.195673000
C	-4.179050000	-0.173937000	-1.013881000
C	-5.510137000	1.719337000	-1.844614000
H	-5.688667000	2.794969000	-1.885189000
C	-3.651154000	-4.687572000	1.135156000
C	-3.308057000	-2.013943000	0.221621000
C	-5.003834000	-1.036090000	-1.792220000
C	-4.075349000	-2.948408000	-0.524280000
C	-4.251073000	-4.254731000	-0.055054000
H	-4.850695000	-4.948668000	-0.646695000
C	-4.625946000	-2.497580000	-1.856748000
C	-2.708992000	-2.452433000	1.438486000
C	-2.874835000	-3.782997000	1.867787000
H	-2.397219000	-4.113244000	2.789710000
C	-6.078797000	-0.520592000	-2.521698000
H	-6.700530000	-1.209986000	-3.095514000
C	-4.443130000	1.225878000	-1.068441000
C	-3.172479000	-1.904661000	4.801445000
H	-3.729610000	-2.691393000	4.275287000
H	-3.812665000	-1.528668000	5.614225000
H	-2.285296000	-2.355839000	5.264665000
C	-6.349061000	0.855948000	-2.554196000
C	-2.818757000	-0.748482000	3.848961000
H	-2.224471000	-0.004283000	4.402819000
C	-4.094393000	-0.058123000	3.333170000
H	-3.846833000	0.779116000	2.667423000
H	-4.688580000	0.326603000	4.175816000
H	-4.717945000	-0.761930000	2.764998000
C	-0.331150000	-2.193685000	3.155854000
H	-0.798180000	-2.928674000	3.829555000
C	-2.692160000	3.396601000	-1.696234000
H	-3.602816000	3.902231000	-2.058827000
C	-4.259125000	3.593795000	0.775766000
H	-4.475739000	4.414792000	0.072648000
C	-3.416873000	4.154527000	1.940874000
H	-3.244789000	3.377214000	2.697442000
H	-3.953946000	4.983414000	2.426016000
H	-2.438152000	4.528558000	1.614685000
C	0.498622000	-2.948114000	2.102488000
H	-0.114240000	-3.661992000	1.539080000
H	1.306312000	-3.506550000	2.599204000
H	0.949054000	-2.249813000	1.387868000
C	0.561194000	-1.258360000	3.996327000
H	1.052044000	-0.514605000	3.353905000
H	1.349281000	-1.842364000	4.494627000
H	-0.002047000	-0.726389000	4.775983000
C	-5.595778000	3.039204000	1.304290000
H	-6.250713000	2.693486000	0.497322000
H	-6.120411000	3.830085000	1.861708000
H	-5.435840000	2.197409000	1.989757000
C	-2.142615000	2.500299000	-2.820986000
H	-1.289776000	1.905910000	-2.465325000
H	-1.785000000	3.121431000	-3.655067000
H	-2.910095000	1.815971000	-3.201788000
C	-1.659753000	4.460096000	-1.281178000
H	-2.054660000	5.153582000	-0.526430000
H	-1.370340000	5.055562000	-2.160025000
H	-0.756086000	3.983534000	-0.881143000
H	-3.783010000	-5.711302000	1.482372000
H	-3.848535000	-2.632874000	-2.634040000
H	-5.482156000	-3.115706000	-2.162825000
H	-7.184635000	1.244374000	-3.134434000
H	-1.226267000	2.389864000	3.410479000
H	0.016541000	-0.639565000	-0.125431000
N	1.356817000	2.274109000	-3.173766000
N	1.352666000	1.648045000	-2.206531000

G(open-shell singlet)

Ti	1.431067000	0.500292000	-0.561634000
P	1.793465000	-1.338466000	-2.312851000
P	2.894541000	2.444931000	0.440076000
N	3.151202000	-0.557802000	0.215224000
C	4.058053000	0.012294000	1.144522000
C	5.112280000	2.004518000	2.146626000
H	5.152547000	3.090483000	2.245912000
C	4.062069000	-4.559365000	-1.021547000
C	3.438772000	-1.897497000	-0.162094000
C	4.933607000	-0.777928000	1.946263000
C	4.267973000	-2.754263000	0.615250000
C	4.582832000	-4.043867000	0.171178000
H	5.232866000	-4.661951000	0.793209000
C	4.735781000	-2.272354000	1.964944000
C	2.898949000	-2.438489000	-1.368222000
C	3.206467000	-3.749510000	-1.774437000
H	2.767409000	-4.138491000	-2.693049000
C	5.902893000	-0.177125000	2.756086000
H	6.566386000	-0.822175000	3.335004000
C	4.143540000	1.428173000	1.304984000
C	2.849834000	-1.931983000	-4.981932000
H	3.313386000	-2.861076000	-4.621733000
H	3.472200000	-1.553071000	-5.807160000
H	1.863206000	-2.172216000	-5.398352000
C	6.018013000	1.215276000	2.859848000
C	2.783813000	-0.870260000	-3.868365000
H	2.263445000	0.017745000	-4.258327000
C	4.205791000	-0.451186000	-3.444169000
H	4.187448000	0.248195000	-2.600107000
H	4.721566000	0.033797000	-4.286288000
H	4.792216000	-1.328249000	-3.139123000
C	0.415630000	-2.440812000	-2.978848000
H	0.885592000	-3.138015000	-3.689641000
C	2.188622000	3.532498000	1.826842000
H	2.987147000	4.244072000	2.096547000
C	4.003139000	3.644214000	-0.529496000
H	4.710702000	4.035075000	0.220170000
C	3.266553000	4.835088000	-1.173569000
H	2.448878000	4.501114000	-1.825005000
H	3.976494000	5.402836000	-1.794062000

H	2.861622000	5.526902000	-0.425348000
C	-0.275644000	-3.265453000	-1.878429000
H	0.431826000	-3.924550000	-1.360478000
H	-1.059288000	-3.891611000	-2.332101000
H	-0.745063000	-2.611799000	-1.133930000
C	-0.603405000	-1.568211000	-3.740336000
H	-1.084586000	-0.859339000	-3.052507000
H	-1.387376000	-2.203176000	-4.179664000
H	-0.139623000	-0.992876000	-4.553849000
C	4.804288000	2.868977000	-1.592396000
H	5.324039000	2.004231000	-1.160706000
H	5.558808000	3.532523000	-2.041064000
H	4.144692000	2.518746000	-2.396015000
C	1.828315000	2.687384000	3.064539000
H	1.053892000	1.951515000	2.807039000
H	1.423671000	3.344101000	3.849975000
H	2.694654000	2.154254000	3.472226000
C	0.939126000	4.313473000	1.371373000
H	1.118620000	4.950503000	0.498528000
H	0.592991000	4.958012000	2.194142000
H	0.136590000	3.609505000	1.118600000
H	4.305225000	-5.569755000	-1.346760000
H	3.972821000	-2.526742000	2.726871000
H	5.657356000	-2.788918000	2.271042000
H	6.775231000	1.668316000	3.497804000
H	0.094627000	1.502185000	0.277262000
Ti	-1.458687000	0.387555000	0.236820000
P	-1.519950000	-1.109022000	2.310965000
P	-3.283360000	2.232963000	-0.354593000
N	-3.194992000	-0.751253000	-0.111772000
C	-4.288393000	-0.303471000	-0.886862000
C	-5.657762000	1.537346000	-1.772392000
H	-5.829687000	2.608602000	-1.887053000
C	-3.673295000	-4.611970000	1.620900000
C	-3.342921000	-2.049775000	0.434598000
C	-5.177879000	-1.213845000	-1.525891000
C	-4.185493000	-3.025063000	-0.160506000
C	-4.354442000	-4.276156000	0.443633000
H	-5.014228000	-5.004346000	-0.031248000
C	-4.824588000	-2.682767000	-1.486342000
C	-2.647229000	-2.392280000	1.630583000
C	-2.812889000	-3.670016000	2.197034000
H	-2.265341000	-3.931614000	3.101902000
C	-6.297290000	-0.742003000	-2.217319000
H	-6.967913000	-1.465747000	-2.683694000
C	-4.542067000	1.092244000	-1.036913000
C	-2.547946000	-1.465232000	5.031810000
H	-3.116184000	-2.352907000	4.721727000
H	-3.097972000	-0.992110000	5.859807000
H	-1.577101000	-1.791935000	5.426081000
C	-6.553666000	0.631439000	-2.346751000
C	-2.408466000	-0.466574000	3.868893000
H	-1.785051000	0.380251000	4.200451000
C	-3.787990000	0.080345000	3.458027000
H	-3.700875000	0.776338000	2.613441000
H	-4.258059000	0.608045000	4.301484000
H	-4.453469000	-0.736781000	3.147798000
C	-0.086964000	-2.105541000	3.029347000
H	-0.511938000	-2.768109000	3.799135000
C	-2.862048000	3.269856000	-1.881349000
H	-3.801570000	3.755045000	-2.194664000
C	-4.179310000	3.510593000	0.741961000
H	-4.407416000	4.358732000	0.075939000
C	-3.227307000	4.000971000	1.853419000
H	-2.974699000	3.180033000	2.538970000
H	-3.711918000	4.796295000	2.439587000
H	-2.288172000	4.399818000	1.450453000
C	0.588310000	-2.972680000	1.952883000
H	-0.111934000	-3.697192000	1.519613000
H	1.426873000	-3.529262000	2.397822000
H	0.981584000	-2.349024000	1.141763000
C	0.929156000	-1.161205000	3.700370000
H	1.387242000	-0.498542000	2.954802000
H	1.733215000	-1.748935000	4.168022000
H	0.472395000	-0.539202000	4.483273000
C	-5.501657000	2.995576000	1.341009000
H	-6.221159000	2.705893000	0.567307000
H	-5.953617000	3.789702000	1.954421000
H	-5.338176000	2.124818000	1.988000000
C	-2.374912000	2.349187000	-3.016207000
H	-1.482986000	1.785747000	-2.708566000
H	-2.095023000	2.950399000	-3.893437000
H	-3.152093000	1.636503000	-3.317772000
C	-1.820780000	4.357859000	-1.559953000
H	-2.174088000	5.057206000	-0.789866000
H	-1.606084000	4.942096000	-2.466925000
H	-0.881163000	3.906390000	-1.217705000
H	-3.803472000	-5.592766000	2.076008000
H	-4.106453000	-2.901407000	-2.300889000
H	-5.708754000	-3.308293000	-1.675135000
H	-7.424808000	0.984015000	-2.896725000
H	-0.007286000	-0.656164000	-0.330587000
N	1.177897000	2.320719000	-3.123497000
N	1.196692000	1.659339000	-2.177990000

G(triplet)

Ti	1.421882000	0.567568000	-0.537431000
P	1.999898000	-0.899217000	-2.586178000
P	2.716299000	2.257043000	0.968859000
N	3.085323000	-0.634479000	0.163821000
C	3.885631000	-0.258172000	1.274978000
C	4.769194000	1.496668000	2.765313000
H	4.760678000	2.538875000	3.088490000
C	4.220116000	-4.300318000	-1.757481000
C	3.448577000	-1.867527000	-0.445494000
C	4.712898000	-1.183285000	1.977165000
C	4.231983000	-2.855088000	0.216514000
C	4.618821000	-4.027332000	-0.444120000
H	5.229174000	-4.750198000	0.100404000
C	4.578146000	-2.652687000	1.669223000
C	3.040490000	-2.160616000	-1.782531000
C	3.416938000	-3.361136000	-2.411023000
H	3.075073000	-3.560445000	-3.426495000
C	5.579111000	-0.749734000	2.986860000
H	6.209525000	-1.490984000	3.481507000
C	3.904556000	1.093850000	1.731592000
C	3.301815000	-0.971887000	-5.205927000
H	3.780077000	-1.934789000	-4.978509000
H	3.967067000	-0.429562000	-5.895166000
H	2.362723000	-1.165763000	-5.739778000
C	5.631886000	0.590893000	3.387847000
C	3.102394000	-0.132126000	-3.930546000
H	2.586329000	0.802930000	-4.196513000
C	4.466436000	0.226277000	-3.307792000
H	4.349620000	0.763371000	-2.359715000
H	5.038726000	0.862208000	-3.999339000
H	5.051252000	-0.681993000	-3.109570000
C	0.711696000	-1.872578000	-3.560428000
H	1.264570000	-2.461169000	-4.308981000
C	1.887538000	3.094437000	2.458198000
H	2.638023000	3.781218000	2.885120000
C	3.897989000	3.615862000	0.356869000
H	4.539691000	3.830441000	1.227443000
C	3.213940000	4.926981000	-0.076413000
H	2.466271000	4.753431000	-0.860772000
H	3.973857000	5.610088000	-0.485836000
H	2.731848000	5.440715000	0.764229000
C	-0.081939000	-2.849204000	-2.672737000

H	0.576041000	-3.565709000	-2.165710000
H	-0.792053000	-3.414387000	-3.295864000
H	-0.654537000	-2.304861000	-1.911055000
C	-0.233416000	-0.900308000	-4.294528000
H	-0.794428000	-0.296860000	-3.569872000
H	-0.954813000	-1.466998000	-4.902145000
H	0.305717000	-0.215314000	-4.963357000
C	4.786764000	3.071128000	-0.775795000
H	5.270307000	2.126742000	-0.494714000
H	5.575437000	3.801934000	-1.010867000
H	4.196685000	2.908758000	-1.686046000
C	1.471077000	2.070207000	3.530974000
H	0.743155000	1.363653000	3.109807000
H	0.990169000	2.596711000	4.370060000
H	2.323967000	1.503578000	3.921798000
C	0.645150000	3.895716000	2.020964000
H	0.866533000	4.662418000	1.269969000
H	0.204938000	4.397201000	2.896767000
H	-0.100328000	3.210275000	1.598783000
H	4.517459000	-5.223653000	-2.252202000
H	3.776109000	-3.084644000	2.299309000
H	5.497323000	-3.196186000	1.933663000
H	6.309032000	0.913146000	4.177391000
H	0.078569000	1.128013000	0.628908000
Ti	-1.480506000	0.171994000	0.089854000
P	-1.542416000	-1.371493000	2.179496000
P	-3.104266000	2.203414000	-0.377760000
N	-3.313380000	-0.788877000	-0.151285000
C	-4.327728000	-0.246880000	-0.974083000
C	-5.437032000	1.711489000	-1.950241000
H	-5.488362000	2.792088000	-2.088175000
C	-4.124826000	-4.591544000	1.580935000
C	-3.567882000	-2.069846000	0.391231000
C	-5.298385000	-1.068134000	-1.610496000
C	-4.519201000	-2.953038000	-0.185781000
C	-4.802774000	-4.179047000	0.426690000
H	-5.549694000	-4.831814000	-0.028374000
C	-5.137405000	-2.568066000	-1.511121000
C	-2.861498000	-2.497016000	1.555488000
C	-3.141668000	-3.754600000	2.121493000
H	-2.585573000	-4.085502000	2.997624000
C	-6.330570000	-0.489309000	-2.356188000
H	-7.071242000	-1.142540000	-2.820611000
C	-4.404177000	1.163400000	-1.166932000
C	-2.368728000	-1.798480000	4.942366000
H	-3.153904000	-2.509214000	4.652120000
H	-2.689491000	-1.311790000	5.875959000
H	-1.451756000	-2.361020000	5.161186000
C	-6.413395000	0.898609000	-2.535027000
C	-2.162787000	-0.730579000	3.853147000
H	-1.369172000	-0.038125000	4.175434000
C	-3.450871000	0.081389000	3.631223000
H	-3.294951000	0.861229000	2.875500000
H	-3.765204000	0.562290000	4.569481000
H	-4.268040000	-0.567480000	3.286733000
C	-0.156724000	-2.563848000	2.636007000
H	-0.582521000	-3.316884000	3.317009000
C	-2.649294000	3.374105000	-1.793846000
H	-3.579303000	3.884510000	-2.093974000
C	-4.068620000	3.369547000	0.788944000
H	-4.376374000	4.215771000	0.152455000
C	-3.159685000	3.906066000	1.912694000
H	-2.810456000	3.089675000	2.558528000
H	-3.722151000	4.617348000	2.536379000
H	-2.275108000	4.422758000	1.523755000
C	0.355697000	-3.275129000	1.369823000
H	-0.439178000	-3.854134000	0.882214000
H	1.172249000	-3.964626000	1.630184000
H	0.748738000	-2.545062000	0.648853000
C	0.981978000	-1.824674000	3.362757000
H	1.433016000	-1.067525000	2.709399000
H	1.768398000	-2.541173000	3.641934000
H	0.641648000	-1.331205000	4.283438000
C	-5.337358000	2.719824000	1.374592000
H	-6.052517000	2.440186000	0.593203000
H	-5.827779000	3.433113000	2.054287000
H	-5.098902000	1.817060000	1.950759000
C	-2.116765000	2.559438000	-2.986731000
H	-1.234744000	1.975032000	-2.691229000
H	-1.811463000	3.237622000	-3.796774000
H	-2.879295000	1.874054000	-3.378190000
C	-1.627464000	4.433823000	-1.340649000
H	-2.039921000	5.103626000	-0.574282000
H	-1.333071000	5.052438000	-2.200930000
H	-0.723133000	3.957204000	-0.942794000
H	-4.344649000	-5.554505000	2.039277000
H	-4.475847000	-2.914769000	-2.329325000
H	-6.100622000	-3.077527000	-1.659263000
H	-7.217953000	1.334983000	-3.124931000
H	-0.145006000	-0.236848000	-1.109409000
N	1.428050000	2.870306000	-2.681165000
N	1.342401000	2.042598000	-1.877944000

G(quintet)

Ti	1.447413000	0.531200000	-0.620377000
P	1.822449000	-1.336304000	-2.334409000
P	2.899632000	2.433795000	0.461750000
N	3.114147000	-0.569148000	0.240345000
C	4.004154000	-0.016142000	1.191969000
C	5.072100000	1.959227000	2.214359000
H	5.130890000	3.044455000	2.312066000
C	3.973662000	-4.594707000	-0.953887000
C	3.382809000	-1.914047000	-0.123574000
C	4.843036000	-0.819819000	2.020136000
C	4.170835000	-2.786548000	0.680745000
C	4.470776000	-4.084002000	0.251422000
H	5.089046000	-4.712682000	0.894864000
C	4.610714000	-2.308878000	2.041166000
C	2.868321000	-2.450088000	-1.343310000
C	3.159019000	-3.770057000	-1.734592000
H	2.737473000	-4.154256000	-2.663292000
C	5.804135000	-0.235342000	2.850521000
H	6.439507000	-0.890948000	3.448821000
C	4.113153000	1.398212000	1.350655000
C	2.967714000	-2.010949000	-4.945780000
H	3.427945000	-2.923245000	-4.541612000
H	3.610577000	-1.653618000	-5.764829000
H	1.995465000	-2.273423000	-5.382367000
C	5.944927000	1.155449000	2.951374000
C	2.859676000	-0.913970000	-3.870490000
H	2.347755000	-0.042759000	-4.307067000
C	4.262882000	-0.469394000	-3.411645000
H	4.207943000	0.270246000	-2.603910000
H	4.810603000	-0.023407000	-4.255092000
H	4.838871000	-1.328052000	-3.041159000
C	0.430297000	-2.410008000	-3.018213000
H	0.897881000	-3.133004000	-3.704444000
C	2.163073000	3.497678000	1.853689000
H	2.964204000	4.188903000	2.165017000
C	4.039437000	3.646015000	-0.454290000
H	4.714845000	4.036909000	0.324382000
C	3.322149000	4.836758000	-1.120320000
H	2.529640000	4.503033000	-1.802151000
H	4.051486000	5.410024000	-1.712521000
H	2.887397000	5.523936000	-0.384707000
C	-0.307887000	-3.194213000	-1.918904000
H	0.369696000	-3.864066000	-1.375539000
H	-1.100294000	-3.805264000	-2.377746000

H	-0.771482000	-2.515039000	-1.193880000
C	-0.544994000	-1.524874000	-3.821800000
H	-1.025946000	-0.789081000	-3.162605000
H	-1.334719000	-2.147042000	-4.268988000
H	-0.045343000	-0.979524000	-4.634794000
C	4.886816000	2.879557000	-1.487865000
H	5.394803000	2.016818000	-1.038656000
H	5.653505000	3.549973000	-1.904505000
H	4.262242000	2.526886000	-2.317842000
C	1.758424000	2.625066000	3.057910000
H	0.984852000	1.902386000	2.760518000
H	1.336003000	3.264563000	3.848151000
H	2.606776000	2.072130000	3.476475000
C	0.937964000	4.310078000	1.389884000
H	1.146224000	4.962722000	0.535279000
H	0.584761000	4.942356000	2.219140000
H	0.128496000	3.627022000	1.104153000
H	4.202973000	-5.612160000	-1.266830000
H	3.820166000	-2.540930000	2.781825000
H	5.510786000	-2.845042000	2.376130000
H	6.695639000	1.596128000	3.605469000
H	0.027914000	1.611558000	-0.004577000
Ti	-1.436398000	0.410319000	0.293980000
P	-1.608862000	-1.125751000	2.343118000
P	-3.240139000	2.256062000	-0.329389000
N	-3.151405000	-0.729647000	-0.159251000
C	-4.214989000	-0.266779000	-0.964783000
C	-5.557643000	1.591089000	-1.853310000
H	-5.730848000	2.664203000	-1.946370000
C	-3.709685000	-4.618430000	1.483343000
C	-3.324990000	-2.035393000	0.358126000
C	-5.075443000	-1.163756000	-1.659637000
C	-4.138467000	-3.000635000	-0.292797000
C	-4.334822000	-4.261546000	0.280816000
H	-4.971244000	-4.981174000	-0.237039000
C	-4.717037000	-2.631820000	-1.639133000
C	-2.689089000	-2.398909000	1.580830000
C	-2.879735000	-3.686688000	2.116900000
H	-2.375971000	-3.963433000	3.042550000
C	-6.169278000	-0.678606000	-2.381942000
H	-6.818222000	-1.392255000	-2.892433000
C	-4.469225000	1.131135000	-1.086280000
C	-2.729729000	-1.539669000	5.018861000
H	-3.268589000	-2.433665000	4.676210000
H	-3.319378000	-1.088842000	5.831843000
H	-1.767858000	-1.853250000	5.444561000
C	-6.425967000	0.697135000	-2.485747000
C	-2.567168000	-0.522397000	3.875131000
H	-1.974066000	0.331952000	4.241803000
C	-3.941208000	0.002064000	3.418181000
H	-3.837796000	0.702327000	2.578920000
H	-4.449694000	0.517439000	4.246750000
H	-4.580243000	-0.825889000	3.082301000
C	-0.193958000	-2.123112000	3.094966000
H	-0.642267000	-2.800773000	3.837956000
C	-2.767457000	3.319829000	-1.825645000
H	-3.703042000	3.794329000	-2.166007000
C	-4.182940000	3.522955000	0.743281000
H	-4.382403000	4.381334000	0.081161000
C	-3.278016000	3.995069000	1.901158000
H	-3.060005000	3.163704000	2.586524000
H	-3.783474000	4.785122000	2.476808000
H	-2.320074000	4.394635000	1.545033000
C	0.525903000	-2.968418000	2.029574000
H	-0.154865000	-3.685152000	1.554465000
H	1.345409000	-3.533457000	2.498830000
H	0.950470000	-2.329516000	1.246801000
C	0.791740000	-1.184321000	3.817516000
H	1.278611000	-0.512292000	3.098980000
H	1.578040000	-1.775551000	4.310222000
H	0.302532000	-0.572323000	4.588736000
C	-5.528822000	3.001605000	1.281038000
H	-6.216340000	2.722356000	0.475106000
H	-6.005709000	3.787400000	1.886389000
H	-5.391802000	2.122054000	1.922441000
C	-2.223434000	2.425927000	-2.955375000
H	-1.324248000	1.886828000	-2.626320000
H	-1.938893000	3.044864000	-3.818916000
H	-2.970108000	1.693670000	-3.285899000
C	-1.755071000	4.419046000	-1.457039000
H	-2.135770000	5.095709000	-0.679757000
H	-1.531362000	5.026902000	-2.346411000
H	-0.815835000	3.974402000	-1.105756000
H	-3.860042000	-5.607450000	1.913752000
H	-3.960276000	-2.827968000	-2.423829000
H	-5.588037000	-3.256718000	-1.882967000
H	-7.276696000	1.061017000	-3.059845000
H	0.048065000	-0.655544000	-0.216159000
N	1.408288000	2.331331000	-3.220118000
N	1.395388000	1.684005000	-2.266989000

$TS_{G2m'}$(open-shell singlet)

Ti	1.408349000	0.350682000	-0.384409000
P	1.819455000	-1.571114000	-2.058896000
P	2.802053000	2.506738000	0.171343000
N	3.318822000	-0.444544000	0.235957000
C	4.220318000	0.287823000	1.050410000
C	5.114689000	2.448636000	1.825284000
H	5.061165000	3.538208000	1.822467000
C	4.648159000	-4.361458000	-0.859333000
C	3.738796000	-1.762049000	-0.085921000
C	5.209209000	-0.346854000	1.856519000
C	4.712547000	-2.462481000	0.678879000
C	5.167442000	-3.722650000	0.273158000
H	5.926721000	-4.220714000	0.878793000
C	5.173326000	-1.849928000	1.978042000
C	3.189194000	-2.434691000	-1.218560000
C	3.640990000	-3.715610000	-1.583800000
H	3.194058000	-4.214046000	-2.443670000
C	6.145384000	0.410535000	2.568317000
H	6.897604000	-0.115475000	3.158899000
C	4.176256000	1.713097000	1.078473000
C	2.894870000	-2.133139000	-4.710398000
H	3.694841000	-2.757969000	-4.290278000
H	3.273607000	-1.691907000	-5.645038000
H	2.047513000	-2.780156000	-4.972398000
C	6.119315000	1.811261000	2.558575000
C	2.500663000	-1.009050000	-3.735744000
H	1.675748000	-0.426103000	-4.173917000
C	3.683260000	-0.052892000	-3.493542000
H	3.389792000	0.771246000	-2.830520000
H	4.027210000	0.375457000	-4.446820000
H	4.527222000	-0.579777000	-3.027227000
C	0.585571000	-2.917677000	-2.511396000
H	1.103735000	-3.609707000	-3.193646000
C	2.166788000	3.760734000	1.441833000
H	3.022279000	4.424570000	1.650648000
C	3.619213000	3.682383000	-1.093567000
H	3.749863000	4.636414000	-0.555726000
C	2.692174000	3.921279000	-2.303604000
H	2.573876000	3.004799000	-2.894094000
H	3.126988000	4.693907000	-2.955881000
H	1.688519000	4.251003000	-2.009074000
C	0.124887000	-3.704451000	-1.271174000
H	0.967764000	-4.196673000	-0.769893000
H	-0.596701000	-4.478250000	-1.572449000
H	-0.367478000	-3.040629000	-0.551374000
C	-0.613481000	-2.295085000	-3.255508000

H	-1.151333000	-1.595201000	-2.602091000
H	-1.314532000	-3.088873000	-3.553954000
H	-0.311473000	-1.755850000	-4.163660000
C	5.006538000	3.200258000	-1.560088000
H	5.717953000	3.128308000	-0.729863000
H	5.406636000	3.910165000	-2.300004000
H	4.948833000	2.214499000	-2.038875000
C	1.738102000	3.082903000	2.755190000
H	0.886033000	2.414582000	2.578293000
H	1.432530000	3.851334000	3.481924000
H	2.555232000	2.499424000	3.197286000
C	1.016230000	4.606026000	0.865770000
H	1.323772000	5.192408000	-0.009890000
H	0.658318000	5.313314000	1.629482000
H	0.178008000	3.959217000	0.575218000
H	5.003809000	-5.346929000	-1.156106000
H	4.466606000	-2.132896000	2.782865000
H	6.154741000	-2.245906000	2.277065000
H	6.851928000	2.387601000	3.121395000
H	0.262321000	1.279374000	0.735926000
Ti	-1.366872000	0.423228000	0.235917000
P	-1.627542000	-1.007127000	2.352654000
P	-3.283076000	2.189911000	-0.373717000
N	-3.022770000	-0.786923000	-0.221560000
C	-4.175495000	-0.383640000	-0.926415000
C	-5.736922000	1.378032000	-1.615364000
H	-5.999517000	2.434665000	-1.671593000
C	-3.101641000	-4.761081000	1.293923000
C	-3.063312000	-2.114996000	0.268668000
C	-5.017160000	-1.332176000	-1.573640000
C	-3.799597000	-3.134038000	-0.387072000
C	-3.815844000	-4.433956000	0.132982000
H	-4.386580000	-5.203323000	-0.389926000
C	-4.520649000	-2.759365000	-1.662577000
C	-2.385401000	-2.433865000	1.481916000
C	-2.395363000	-3.754940000	1.965383000
H	-1.860441000	-3.997413000	2.883305000
C	-6.215445000	-0.921838000	-2.163719000
H	-6.850716000	-1.670286000	-2.640508000
C	-4.537994000	0.995621000	-0.981459000
C	-3.021952000	-1.601908000	4.860594000
H	-3.243445000	-2.614597000	4.495142000
H	-3.843131000	-1.305740000	5.531349000
H	-2.104081000	-1.639844000	5.460987000
C	-6.593616000	0.429694000	-2.181760000
C	-2.929206000	-0.603400000	3.691636000
H	-2.616795000	0.376937000	4.087111000
C	-4.309456000	-0.447188000	3.023342000
H	-4.259761000	0.178669000	2.123621000
H	-5.022504000	0.004787000	3.728922000
H	-4.701653000	-1.426887000	2.719881000
C	-0.212959000	-1.718270000	3.377839000
H	-0.661812000	-2.459787000	4.056518000
C	-3.254622000	3.492037000	-1.762423000
H	-4.219631000	4.019851000	-1.671274000
C	-4.032530000	3.280527000	1.015037000
H	-4.000913000	4.300447000	0.600881000
C	-3.118799000	3.246763000	2.256201000
H	-3.089795000	2.241840000	2.697962000
H	-3.490446000	3.944218000	3.022716000
H	-2.087374000	3.530300000	2.006305000
C	0.854017000	-2.426385000	2.525639000
H	0.425719000	-3.235402000	1.921992000
H	1.618908000	-2.859359000	3.189136000
H	1.347018000	-1.721372000	1.845328000
C	0.420955000	-0.595496000	4.225289000
H	0.871237000	0.165466000	3.574860000
H	1.215668000	-1.011095000	4.862492000
H	-0.308641000	-0.099712000	4.881120000
C	-5.494173000	2.963057000	1.377408000
H	-6.169578000	3.098316000	0.524552000
H	-5.824955000	3.639041000	2.180855000
H	-5.610226000	1.932338000	1.733122000
C	-3.153905000	2.894812000	-3.177349000
H	-2.215205000	2.344005000	-3.309030000
H	-3.169520000	3.713272000	-3.913446000
H	-3.991174000	2.222489000	-3.397281000
C	-2.116840000	4.502527000	-1.514391000
H	-2.162366000	4.954161000	-0.513372000
H	-2.176942000	5.317954000	-2.250571000
H	-1.140950000	4.014264000	-1.627706000
H	-3.108424000	-5.780244000	1.677896000
H	-3.821349000	-2.840511000	-2.516790000
H	-5.347208000	-3.454247000	-1.868997000
H	-7.526100000	0.737489000	-2.652420000
H	0.039312000	-0.810740000	0.083664000
N	-0.011511000	1.627809000	-2.873925000
N	0.459551000	1.187151000	-1.906128000

$TS_{G2m'}$(triplet)

Ti	1.395375000	0.400005000	-0.450711000
P	1.814974000	-1.493328000	-2.152505000
P	2.813242000	2.492384000	0.240786000
N	3.259119000	-0.467630000	0.221587000
C	4.137729000	0.211675000	1.105092000
C	5.035079000	2.322446000	2.006468000
H	5.003191000	3.412263000	2.042934000
C	4.547529000	-4.377370000	-0.956811000
C	3.664221000	-1.783322000	-0.128976000
C	5.079346000	-0.472889000	1.926869000
C	4.594580000	-2.531028000	0.645797000
C	5.038333000	-3.786489000	0.213578000
H	5.765039000	-4.320010000	0.828971000
C	5.019501000	-1.978593000	1.983291000
C	3.140260000	-2.409770000	-1.299820000
C	3.578490000	-3.687283000	-1.692188000
H	3.148967000	-4.148357000	-2.581281000
C	5.993518000	0.237299000	2.712493000
H	6.708672000	-0.326808000	3.313909000
C	4.120035000	1.635202000	1.188234000
C	2.933721000	-2.030985000	-4.791677000
H	3.713110000	-2.680965000	-4.371211000
H	3.337478000	-1.579962000	-5.711044000
H	2.077309000	-2.654293000	-5.080506000
C	5.991686000	1.637201000	2.760526000
C	2.547256000	-0.916931000	-3.802507000
H	1.748035000	-0.303949000	-4.246725000
C	3.748292000	0.003894000	-3.516451000
H	3.460659000	0.824789000	-2.847005000
H	4.125183000	0.438100000	-4.454489000
H	4.567267000	-0.552777000	-3.040220000
C	0.550486000	-2.794393000	-2.655744000
H	1.057242000	-3.483442000	-3.349539000
C	2.153223000	3.729867000	1.516041000
H	3.016247000	4.362215000	1.783215000
C	3.736278000	3.676430000	-0.941361000
H	3.889383000	4.601083000	-0.359692000
C	2.878290000	4.007328000	-2.180232000
H	2.754546000	3.124713000	-2.818761000
H	3.373677000	4.791041000	-2.773490000
H	1.874305000	4.362954000	-1.919021000
C	0.051391000	-3.599661000	-1.442506000
H	0.872809000	-4.130675000	-0.945392000
H	-0.688922000	-4.343272000	-1.773579000
H	-0.429525000	-2.941013000	-0.709982000
C	-0.620983000	-2.117144000	-3.396206000
H	-1.140489000	-1.414757000	-2.730412000
H	-1.345036000	-2.880241000	-3.719134000

H	-0.292900000	-1.566976000	-4.288643000
C	5.117295000	3.142809000	-1.369350000
H	5.789626000	3.007965000	-0.514771000
H	5.581037000	3.856383000	-2.067434000
H	5.031310000	2.177755000	-1.885035000
C	1.645164000	3.029931000	2.788898000
H	0.791020000	2.382297000	2.553928000
H	1.317587000	3.787109000	3.518024000
H	2.427699000	2.420379000	3.257233000
C	1.055903000	4.626476000	0.914277000
H	1.419828000	5.225411000	0.069462000
H	0.687024000	5.324665000	1.681228000
H	0.211461000	4.015164000	0.570565000
H	4.893443000	-5.360140000	-1.273399000
H	4.283778000	-2.285339000	2.752550000
H	5.985449000	-2.400554000	2.297201000
H	6.706866000	2.176277000	3.379897000
H	0.217182000	1.367520000	0.609088000
Ti	-1.396124000	0.425973000	0.262945000
P	-1.569814000	-1.049922000	2.347104000
P	-3.304004000	2.194240000	-0.360447000
N	-3.066472000	-0.779242000	-0.182606000
C	-4.211208000	-0.371421000	-0.899956000
C	-5.746635000	1.402638000	-1.625695000
H	-5.994687000	2.462349000	-1.693442000
C	-3.192947000	-4.752602000	1.342044000
C	-3.113131000	-2.108505000	0.304045000
C	-5.057921000	-1.314410000	-1.549466000
C	-3.868988000	-3.120158000	-0.342501000
C	-3.907979000	-4.416474000	0.184470000
H	-4.496650000	-5.176626000	-0.331945000
C	-4.579824000	-2.747670000	-1.623475000
C	-2.418033000	-2.441384000	1.504219000
C	-2.452585000	-3.759775000	1.995009000
H	-1.907222000	-4.009830000	2.904707000
C	-6.244670000	-0.895356000	-2.156753000
H	-6.882490000	-1.641748000	-2.633353000
C	-4.560302000	1.010438000	-0.975005000
C	-2.827505000	-1.573256000	4.942297000
H	-3.103168000	-2.582989000	4.606753000
H	-3.595476000	-1.241982000	5.658119000
H	-1.875409000	-1.633081000	5.484767000
C	-6.608240000	0.459694000	-2.193201000
C	-2.776007000	-0.593803000	3.755082000
H	-2.413698000	0.382810000	4.116252000
C	-4.187254000	-0.405972000	3.164057000
H	-4.168794000	0.204663000	2.252573000
H	-4.845702000	0.078197000	3.900596000
H	-4.624481000	-1.377581000	2.898534000
C	-0.125282000	-1.824404000	3.280129000
H	-0.559317000	-2.536130000	3.999105000
C	-3.210514000	3.458976000	-1.774967000
H	-4.185917000	3.974865000	-1.758121000
C	-4.070135000	3.306233000	0.997836000
H	-4.116508000	4.307470000	0.541341000
C	-3.113036000	3.375616000	2.205437000
H	-3.008107000	2.390353000	2.681081000
H	-3.500609000	4.076860000	2.960294000
H	-2.110189000	3.711340000	1.909212000
C	0.835716000	-2.590285000	2.355107000
H	0.325299000	-3.391826000	1.808084000
H	1.637853000	-3.042509000	2.958674000
H	1.294324000	-1.916006000	1.622037000
C	0.624722000	-0.726542000	4.062295000
H	1.068132000	-0.000322000	3.368634000
H	1.438901000	-1.175315000	4.650478000
H	-0.030339000	-0.182752000	4.757881000
C	-5.495209000	2.914445000	1.427536000
H	-6.204117000	2.954251000	0.592619000
H	-5.844202000	3.611894000	2.204364000
H	-5.529581000	1.900735000	1.844042000
C	-3.021018000	2.810333000	-3.158012000
H	-2.057922000	2.289499000	-3.225989000
H	-3.026195000	3.597028000	-3.927757000
H	-3.825078000	2.101823000	-3.389106000
C	-2.101667000	4.492926000	-1.496924000
H	-2.213833000	4.980327000	-0.518183000
H	-2.127385000	5.279661000	-2.265423000
H	-1.114581000	4.015808000	-1.534128000
H	-3.220052000	-5.768497000	1.733586000
H	-3.876978000	-2.845702000	-2.473343000
H	-5.414024000	-3.433884000	-1.828100000
H	-7.531320000	0.773156000	-2.678300000
H	0.012188000	-0.754714000	-0.032437000
N	0.269660000	1.782265000	-3.033650000
N	0.615760000	1.297154000	-2.037162000

$TS_{G2m'}$(quintet)

Ti	1.435078000	0.321766000	-0.355680000
P	2.047706000	-1.543712000	-2.019690000
P	2.732973000	2.551123000	0.026973000
N	3.326094000	-0.350852000	0.363078000
C	4.200314000	0.466611000	1.116486000
C	5.028998000	2.702173000	1.716750000
H	4.949552000	3.786667000	1.630074000
C	4.805675000	-4.260232000	-0.496978000
C	3.804591000	-1.660544000	0.108330000
C	5.188742000	-0.082462000	1.981565000
C	4.766223000	-2.288463000	0.945373000
C	5.264067000	-3.556631000	0.624537000
H	6.009145000	-4.007211000	1.282644000
C	5.172529000	-1.574937000	2.212983000
C	3.333735000	-2.383279000	-1.027594000
C	3.829813000	-3.669785000	-1.307576000
H	3.447088000	-4.214803000	-2.170341000
C	6.095288000	0.752467000	2.642331000
H	6.850239000	0.297965000	3.286299000
C	4.122823000	1.886402000	1.013034000
C	3.229172000	-2.199157000	-4.618474000
H	3.898922000	-2.935990000	-4.153705000
H	3.745653000	-1.795565000	-5.502958000
H	2.329132000	-2.718702000	-4.971485000
C	6.032616000	2.147737000	2.516493000
C	2.907149000	-1.051123000	-3.644493000
H	2.188976000	-0.366978000	-4.124411000
C	4.182110000	-0.256894000	-3.304041000
H	3.971006000	0.532743000	-2.571740000
H	4.596668000	0.206487000	-4.211670000
H	4.946897000	-0.916979000	-2.872751000
C	0.863093000	-2.909711000	-2.548904000
H	1.435930000	-3.601106000	-3.186548000
C	2.033091000	3.883877000	1.183185000
H	2.836752000	4.632240000	1.288021000
C	3.472757000	3.672815000	-1.336793000
H	3.418809000	4.697806000	-0.934614000
C	2.597860000	3.597827000	-2.605339000
H	2.615574000	2.585652000	-3.030973000
H	2.976858000	4.297949000	-3.365523000
H	1.548990000	3.849106000	-2.402699000
C	0.317465000	-3.695158000	-1.342993000
H	1.123172000	-4.191767000	-0.787821000
H	-0.385268000	-4.465998000	-1.692654000
H	-0.218731000	-3.030968000	-0.655379000
C	-0.283322000	-2.301600000	-3.383348000
H	-0.883551000	-1.615870000	-2.771410000
H	-0.944648000	-3.103200000	-3.745254000
H	0.082635000	-1.748448000	-4.259805000
C	4.945392000	3.363148000	-1.664298000

H	5.599639000	3.502961000	-0.796381000
H	5.288133000	4.033335000	-2.467523000
H	5.071923000	2.330513000	-2.012692000
C	1.685633000	3.335738000	2.578279000
H	0.900757000	2.572360000	2.503573000
H	1.315035000	4.156232000	3.212190000
H	2.559162000	2.890485000	3.069996000
C	0.806582000	4.558849000	0.544422000
H	1.037574000	5.023381000	-0.423815000
H	0.423624000	5.348354000	1.209110000
H	0.008112000	3.820154000	0.392311000
H	5.192502000	-5.251973000	-0.726733000
H	4.441674000	-1.809106000	3.011717000
H	6.148758000	-1.930715000	2.572806000
H	6.740446000	2.785830000	3.043429000
H	0.289399000	1.152705000	0.905575000
Ti	-1.379720000	0.459821000	0.248571000
P	-1.701930000	-1.049675000	2.322200000
P	-3.394742000	2.144703000	-0.326065000
N	-2.964358000	-0.820991000	-0.300804000
C	-4.135465000	-0.452274000	-0.986261000
C	-5.818607000	1.234349000	-1.562092000
H	-6.154549000	2.271261000	-1.556684000
C	-2.830716000	-4.850514000	1.042391000
C	-2.937544000	-2.165685000	0.132873000
C	-4.917232000	-1.418704000	-1.682026000
C	-3.595310000	-3.197410000	-0.583947000
C	-3.539746000	-4.517181000	-0.121286000
H	-4.048752000	-5.297209000	-0.690089000
C	-4.317987000	-2.799011000	-1.851530000
C	-2.280075000	-2.493542000	1.354537000
C	-2.213222000	-3.832708000	1.780455000
H	-1.690374000	-4.080823000	2.703978000
C	-6.147439000	-1.059856000	-2.236740000
H	-6.736008000	-1.820758000	-2.752195000
C	-4.584890000	0.902579000	-0.965427000
C	-3.180537000	-1.895055000	4.697406000
H	-3.297100000	-2.897176000	4.261637000
H	-4.059409000	-1.705975000	5.332701000
H	-2.297547000	-1.896992000	5.349124000
C	-6.617588000	0.261942000	-2.169852000
C	-3.105822000	-0.821250000	3.595559000
H	-2.895073000	0.152555000	4.066439000
C	-4.455902000	-0.730662000	2.856690000
H	-4.415059000	-0.040442000	2.004980000
H	-5.240984000	-0.390150000	3.548213000
H	-4.746511000	-1.714946000	2.466695000
C	-0.281424000	-1.657539000	3.398583000
H	-0.684832000	-2.474780000	4.016274000
C	-3.511216000	3.532266000	-1.633640000
H	-4.489456000	4.003402000	-1.434148000
C	-4.162786000	3.124910000	1.135217000
H	-4.100418000	4.174270000	0.807202000
C	-3.279735000	2.976439000	2.389360000
H	-3.270927000	1.939002000	2.747867000
H	-3.660087000	3.611865000	3.204036000
H	-2.239879000	3.269195000	2.186091000
C	0.897515000	-2.208124000	2.578945000
H	0.584427000	-2.998308000	1.886505000
H	1.651955000	-2.625941000	3.263670000
H	1.374789000	-1.413955000	1.991441000
C	0.182264000	-0.517340000	4.329998000
H	0.568011000	0.325422000	3.740982000
H	0.992808000	-0.874447000	4.982396000
H	-0.626372000	-0.145917000	4.975169000
C	-5.639413000	2.811898000	1.433672000
H	-6.288808000	3.044649000	0.580955000
H	-5.977628000	3.418483000	2.287888000
H	-5.788608000	1.755390000	1.687154000
C	-3.494114000	3.056651000	-3.097611000
H	-2.541368000	2.580332000	-3.347895000
H	-3.624923000	3.930449000	-3.754798000
H	-4.302785000	2.348219000	-3.309219000
C	-2.407559000	4.581782000	-1.396394000
H	-2.385831000	4.950944000	-0.361433000
H	-2.569586000	5.447861000	-2.055493000
H	-1.423136000	4.157162000	-1.628649000
H	-2.777385000	-5.885009000	1.378682000
H	-3.597537000	-2.773041000	-2.691629000
H	-5.087431000	-3.536886000	-2.119519000
H	-7.576277000	0.531089000	-2.610669000
H	-0.005047000	-0.847521000	0.021955000
N	-0.630713000	1.500857000	-2.442010000
N	0.158419000	1.087831000	-1.690870000

2m'(closed-shell singlet)

Ti	1.387018000	0.206233000	-0.461268000
P	2.121831000	-1.920594000	-1.711858000
P	2.380779000	2.601144000	-0.236181000
N	3.435408000	-0.132018000	0.268429000
C	4.201792000	0.869441000	0.917095000
C	4.703124000	3.254253000	1.277547000
H	4.455423000	4.300558000	1.094943000
C	5.389679000	-3.924102000	-0.130649000
C	4.064515000	-1.401484000	0.181156000
C	5.295336000	0.566967000	1.778111000
C	5.149233000	-1.780842000	1.022396000
C	5.803669000	-3.004600000	0.840221000
H	6.640664000	-3.247312000	1.497477000
C	5.519699000	-0.872143000	2.167292000
C	3.627712000	-2.361151000	-0.783397000
C	4.283103000	-3.598164000	-0.920944000
H	3.917555000	-4.317004000	-1.653853000
C	6.091201000	1.587840000	2.309320000
H	6.930065000	1.311699000	2.950748000
C	3.899029000	2.247612000	0.713518000
C	3.287375000	-2.800774000	-4.227992000
H	4.203980000	-3.142063000	-3.728319000
H	3.555997000	-2.507833000	-5.254341000
H	2.592026000	-3.647672000	-4.297930000
C	5.818063000	2.938600000	2.059550000
C	2.675706000	-1.594382000	-3.493711000
H	1.750232000	-1.288750000	-4.006046000
C	3.645907000	-0.398750000	-3.499585000
H	3.185328000	0.485367000	-3.040295000
H	3.923652000	-0.137780000	-4.531628000
H	4.564374000	-0.632681000	-2.944020000
C	1.134741000	-3.511254000	-1.827242000
H	1.777275000	-4.254580000	-2.324851000
C	1.589137000	3.996098000	0.770264000
H	2.350770000	4.793541000	0.788599000
C	2.937545000	3.591674000	-1.774082000
H	2.899104000	4.647296000	-1.457017000
C	1.949045000	3.396161000	-2.943354000
H	2.003839000	2.373743000	-3.337767000
H	2.201285000	4.090546000	-3.759512000
H	0.906786000	3.566309000	-2.650060000
C	0.774255000	-4.032295000	-0.424477000
H	1.673932000	-4.234929000	0.170586000
H	0.201277000	-4.966592000	-0.512068000
H	0.156145000	-3.304300000	0.113946000
C	-0.120469000	-3.282694000	-2.691875000
H	-0.751546000	-2.497245000	-2.256364000
H	-0.707189000	-4.211873000	-2.741216000
H	0.130743000	-2.991136000	-3.720837000
C	4.381986000	3.280044000	-2.211030000
H	5.109858000	3.530075000	-1.430687000
H	4.623327000	3.865306000	-3.111526000

H	4.509625000	2.218385000	-2.458100000
C	1.284637000	3.576667000	2.216936000
H	0.502278000	2.808623000	2.228753000
H	0.925024000	4.449472000	2.783269000
H	2.172171000	3.178663000	2.724557000
C	0.323835000	4.541459000	0.085445000
H	0.535065000	4.974037000	-0.900922000
H	-0.118113000	5.333990000	0.708606000
H	-0.422476000	3.745930000	-0.044535000
H	5.901255000	-4.877589000	-0.251973000
H	4.885995000	-1.114933000	3.043256000
H	6.559224000	-1.039489000	2.484964000
H	6.445080000	3.722792000	2.480942000
H	0.357673000	0.981962000	0.873008000
Ti	-1.279616000	0.506437000	-0.109114000
P	-1.631866000	-0.507140000	2.428800000
P	-3.594817000	1.841626000	-0.579358000
N	-2.681416000	-0.992644000	-0.270881000
C	-3.894243000	-0.892043000	-0.996298000
C	-5.762191000	0.431336000	-1.849364000
H	-6.238695000	1.398476000	-2.007049000
C	-2.226466000	-4.606414000	1.899073000
C	-2.538345000	-2.206167000	0.443450000
C	-4.511415000	-2.057622000	-1.525315000
C	-3.052240000	-3.423267000	-0.067330000
C	-2.896642000	-4.605071000	0.667582000
H	-3.295369000	-5.536744000	0.262982000
C	-3.755948000	-3.365305000	-1.406064000
C	-1.938162000	-2.186822000	1.732579000
C	-1.760634000	-3.395777000	2.430251000
H	-1.274411000	-3.394210000	3.405214000
C	-5.747800000	-1.962166000	-2.170755000
H	-6.209336000	-2.869003000	-2.564935000
C	-4.535251000	0.368089000	-1.160311000
C	-3.111055000	-1.202755000	4.872426000
H	-3.065730000	-2.269712000	4.614261000
H	-4.041646000	-1.039679000	5.437608000
H	-2.274255000	-0.968454000	5.542511000
C	-6.381300000	-0.722636000	-2.340705000
C	-3.127580000	-0.328634000	3.604387000
H	-3.104594000	0.729863000	3.908934000
C	-4.423530000	-0.586179000	2.811203000
H	-4.426399000	-0.063180000	1.847297000
H	-5.296163000	-0.253436000	3.392617000
H	-4.539651000	-1.658097000	2.604022000
C	-0.215406000	-0.762629000	3.649534000
H	-0.549283000	-1.556614000	4.335547000
C	-3.768333000	3.003924000	-2.082759000
H	-4.835103000	3.290000000	-2.061972000
C	-4.698721000	2.862099000	0.622585000
H	-4.831786000	3.819467000	0.095316000
C	-3.919122000	3.158655000	1.918790000
H	-3.731212000	2.241175000	2.489524000
H	-4.492619000	3.846586000	2.559267000
H	-2.945623000	3.621146000	1.705394000
C	1.085263000	-1.230841000	2.975176000
H	0.935839000	-2.145270000	2.388770000
H	1.843842000	-1.434446000	3.747417000
H	1.482746000	-0.456707000	2.306037000
C	0.019682000	0.518169000	4.476047000
H	0.364804000	1.336108000	3.832933000
H	0.796489000	0.334405000	5.233068000
H	-0.885927000	0.852413000	5.000953000
C	-6.101755000	2.301474000	0.917460000
H	-6.716202000	2.233186000	0.012165000
H	-6.619679000	2.969332000	1.623416000
H	-6.061294000	1.302764000	1.367244000
C	-3.471650000	2.361990000	-3.451079000
H	-2.417315000	2.075925000	-3.517121000
H	-3.694841000	3.095649000	-4.242092000
H	-4.089821000	1.473954000	-3.629740000
C	-2.921307000	4.277543000	-1.889205000
H	-3.104066000	4.767477000	-0.921717000
H	-3.161412000	5.005172000	-2.679555000
H	-1.857801000	4.025200000	-1.956506000
H	-2.090038000	-5.535753000	2.450428000
H	-3.009578000	-3.422448000	-2.219059000
H	-4.429478000	-4.224164000	-1.535816000
H	-7.336774000	-0.657513000	-2.859288000
H	0.039411000	-0.853129000	0.182725000
N	-1.002542000	1.607080000	-1.688414000
N	0.074163000	0.925107000	-1.538339000

2m'(triplet)

Ti	1.395710000	0.294421000	-0.407986000
P	2.047768000	-1.727977000	-1.897415000
P	2.623241000	2.582887000	-0.105735000
N	3.346459000	-0.285305000	0.345699000
C	4.207722000	0.607931000	1.024791000
C	4.985187000	2.905070000	1.449976000
H	4.865216000	3.978271000	1.295759000
C	4.929902000	-4.211917000	-0.237289000
C	3.855339000	-1.598688000	0.189401000
C	5.238097000	0.153249000	1.897683000
C	4.855612000	-2.133932000	1.047327000
C	5.387794000	-3.406913000	0.813711000
H	6.161004000	-3.779976000	1.487646000
C	5.269721000	-1.315294000	2.245798000
C	3.385854000	-2.428219000	-0.873205000
C	3.917109000	-3.716770000	-1.065114000
H	3.530498000	-4.339249000	-1.871799000
C	6.141540000	1.057117000	2.465025000
H	6.928470000	0.669123000	3.114182000
C	4.078880000	2.016807000	0.840893000
C	3.318290000	-2.515331000	-4.400671000
H	4.087365000	-3.085054000	-3.861379000
H	3.767142000	-2.157259000	-5.339695000
H	2.499631000	-3.196677000	-4.665974000
C	6.036631000	2.437531000	2.243087000
C	2.838688000	-1.311044000	-3.570488000
H	2.036598000	-0.792559000	-4.119162000
C	3.989900000	-0.314871000	-3.338826000
H	3.649904000	0.555316000	-2.762835000
H	4.385200000	0.040776000	-4.301895000
H	4.810568000	-0.786515000	-2.781405000
C	0.905797000	-3.169106000	-2.286200000
H	1.497413000	-3.894145000	-2.867018000
C	1.919278000	3.928665000	1.029721000
H	2.707693000	4.698394000	1.081313000
C	3.244048000	3.663403000	-1.554638000
H	3.192912000	4.700447000	-1.184180000
C	2.288625000	3.527374000	-2.759358000
H	2.311160000	2.507789000	-3.165889000
H	2.591505000	4.222323000	-3.557259000
H	1.247006000	3.745529000	-2.492370000
C	0.411430000	-3.858721000	-1.001916000
H	1.245741000	-4.268747000	-0.419066000
H	-0.264192000	-4.685454000	-1.265053000
H	-0.141982000	-3.156639000	-0.368175000
C	-0.270705000	-2.680629000	-3.156300000
H	-0.877788000	-1.944881000	-2.613394000
H	-0.915774000	-3.533814000	-3.413728000
H	0.066158000	-2.221710000	-4.096311000
C	4.700160000	3.373614000	-1.964753000
H	5.403461000	3.558763000	-1.145015000
H	4.974904000	4.022421000	-2.810310000
H	4.830391000	2.332524000	-2.285294000
C	1.640394000	3.410379000	2.450686000

H	0.865078000	2.634645000	2.425019000
H	1.280750000	4.240274000	3.078093000
H	2.540544000	2.992002000	2.917237000
C	0.651643000	4.552960000	0.422938000
H	0.832030000	5.001317000	-0.563076000
H	0.273712000	5.346521000	1.085251000
H	-0.132788000	3.790729000	0.320726000
H	5.343051000	-5.206523000	-0.397652000
H	4.564000000	-1.505381000	3.078063000
H	6.263511000	-1.616034000	2.607557000
H	6.743666000	3.130250000	2.696774000
H	0.288951000	1.152924000	0.846461000
Ti	-1.249749000	0.473738000	-0.041259000
P	-1.681887000	-0.780613000	2.346481000
P	-3.399834000	2.051865000	-0.407520000
N	-2.812152000	-0.910023000	-0.336363000
C	-4.010774000	-0.612325000	-0.999589000
C	-5.748175000	0.977348000	-1.664020000
H	-6.118593000	2.000426000	-1.724206000
C	-2.582721000	-4.749579000	1.422767000
C	-2.757008000	-2.190003000	0.239209000
C	-4.775185000	-1.653347000	-1.602770000
C	-3.400915000	-3.300684000	-0.362108000
C	-3.310460000	-4.561770000	0.236321000
H	-3.802356000	-5.411691000	-0.239927000
C	-4.142532000	-3.030981000	-1.654397000
C	-2.104766000	-2.356553000	1.494859000
C	-1.997800000	-3.643663000	2.054388000
H	-1.472962000	-3.783641000	2.999313000
C	-6.016236000	-1.369376000	-2.173817000
H	-6.590056000	-2.181233000	-2.624247000
C	-4.505234000	0.725701000	-1.046644000
C	-3.227584000	-1.622391000	4.692584000
H	-3.259343000	-2.650651000	4.306817000
H	-4.148255000	-1.458404000	5.273570000
H	-2.381538000	-1.534063000	5.386145000
C	-6.516319000	-0.056713000	-2.206425000
C	-3.164638000	-0.602652000	3.539926000
H	-3.046206000	0.404272000	3.971090000
C	-4.477988000	-0.642877000	2.734160000
H	-4.444546000	0.010283000	1.853697000
H	-5.319700000	-0.329729000	3.369937000
H	-4.679645000	-1.661916000	2.378799000
C	-0.290148000	-1.213666000	3.541573000
H	-0.668194000	-2.036267000	4.168235000
C	-3.519637000	3.370799000	-1.787321000
H	-4.515053000	3.821463000	-1.627928000
C	-4.300743000	3.077115000	0.946531000
H	-4.251467000	4.105240000	0.554549000
C	-3.497100000	3.051591000	2.260507000
H	-3.500422000	2.051636000	2.709294000
H	-3.937024000	3.751119000	2.988250000
H	-2.449236000	3.338154000	2.097119000
C	0.987006000	-1.699488000	2.836637000
H	0.790397000	-2.541046000	2.161656000
H	1.718220000	-2.024945000	3.593514000
H	1.444691000	-0.895135000	2.247583000
C	0.012747000	-0.006781000	4.454237000
H	0.372778000	0.844030000	3.861580000
H	0.799348000	-0.272637000	5.176038000
H	-0.867359000	0.320140000	5.025101000
C	-5.784060000	2.739422000	1.180585000
H	-6.391576000	2.911708000	0.283942000
H	-6.183444000	3.379875000	1.982264000
H	-5.922940000	1.694000000	1.481293000
C	-3.459347000	2.848187000	-3.234793000
H	-2.477436000	2.418959000	-3.456154000
H	-3.641549000	3.691401000	-3.919881000
H	-4.219951000	2.083221000	-3.427955000
C	-2.455092000	4.463931000	-1.570697000
H	-2.467093000	4.875338000	-0.551325000
H	-2.627069000	5.297344000	-2.268605000
H	-1.454340000	4.058486000	-1.764678000
H	-2.495736000	-5.742170000	1.862707000
H	-3.426661000	-3.059344000	-2.497896000
H	-4.895194000	-3.807254000	-1.852133000
H	-7.479626000	0.155870000	-2.667797000
H	0.062802000	-0.870923000	0.166852000
N	-1.099390000	1.142234000	-2.043104000
N	0.015055000	0.856378000	-1.620581000

2m'(quintet)

Ti	1.393668000	0.453644000	-0.428275000
P	2.240784000	-1.077161000	-2.361821000
P	2.886531000	2.440633000	0.371110000
N	3.057901000	-0.545697000	0.409102000
C	3.963184000	0.053128000	1.306899000
C	5.041685000	2.061704000	2.214854000
H	5.122842000	3.148463000	2.257712000
C	3.950858000	-4.529186000	-0.773706000
C	3.374679000	-1.868114000	0.029810000
C	4.775983000	-0.730313000	2.174540000
C	4.106778000	-2.738252000	0.878524000
C	4.391706000	-4.044874000	0.465828000
H	4.951686000	-4.698092000	1.137277000
C	4.503526000	-2.217213000	2.241127000
C	2.981067000	-2.340496000	-1.256705000
C	3.251125000	-3.669899000	-1.629595000
H	2.926751000	-4.033861000	-2.604126000
C	5.730681000	-0.115670000	2.989537000
H	6.350062000	-0.740299000	3.635616000
C	4.095970000	1.472782000	1.352920000
C	4.134013000	-1.720866000	-4.495051000
H	4.460246000	-2.618378000	-3.951496000
H	4.990548000	-1.361565000	-5.086020000
H	3.343881000	-2.008663000	-5.200427000
C	5.879658000	1.279628000	3.015395000
C	3.687235000	-0.620550000	-3.515069000
H	3.310963000	0.242657000	-4.088006000
C	4.877692000	-0.155155000	-2.655704000
H	4.562078000	0.567683000	-1.893053000
H	5.644973000	0.312608000	-3.290492000
H	5.335656000	-1.007067000	-2.135424000
C	1.083594000	-2.030374000	-3.505042000
H	1.687351000	-2.835689000	-3.952814000
C	2.228338000	3.640643000	1.690857000
H	3.095462000	4.256237000	1.984603000
C	3.827563000	3.693298000	-0.733385000
H	3.736128000	4.662145000	-0.216647000
C	3.104584000	3.795707000	-2.092753000
H	3.158116000	2.840212000	-2.633619000
H	3.573360000	4.571982000	-2.716816000
H	2.041544000	4.046038000	-1.974515000
C	-0.086912000	-2.675378000	-2.738609000
H	0.264979000	-3.319533000	-1.923408000
H	-0.682175000	-3.288345000	-3.433188000
H	-0.743773000	-1.911740000	-2.304892000
C	0.568846000	-1.124383000	-4.644803000
H	-0.049495000	-0.308643000	-4.250729000
H	-0.054514000	-1.717251000	-5.330767000
H	1.386434000	-0.686231000	-5.233570000
C	5.325496000	3.395736000	-0.925677000
H	5.872557000	3.385278000	0.023722000
H	5.769684000	4.170644000	-1.569253000
H	5.485178000	2.426013000	-1.411892000
C	1.695671000	2.907432000	2.934336000
H	0.860874000	2.248016000	2.663128000
H	1.333487000	3.644538000	3.667841000

H	2.475043000	2.302802000	3.413765000
C	1.143672000	4.555559000	1.097425000
H	1.495783000	5.120498000	0.223108000
H	0.810947000	5.284174000	1.852434000
H	0.276856000	3.955965000	0.793836000
H	4.160745000	-5.555208000	-1.072648000
H	3.675184000	-2.396058000	2.953753000
H	5.374021000	-2.761782000	2.634615000
H	6.620633000	1.745688000	3.663227000
H	0.143076000	1.057698000	0.889301000
Ti	-1.346552000	0.212064000	0.024403000
P	-1.699624000	-1.289012000	2.126699000
P	-3.139533000	2.237397000	-0.203462000
N	-3.150105000	-0.777916000	-0.342359000
C	-4.253071000	-0.202739000	-0.999236000
C	-5.629007000	1.750152000	-1.532963000
H	-5.790638000	2.827681000	-1.500289000
C	-3.687182000	-4.777185000	0.974613000
C	-3.327931000	-2.118206000	0.073361000
C	-5.187189000	-1.013557000	-1.702809000
C	-4.182557000	-3.003980000	-0.628708000
C	-4.358730000	-4.313235000	-0.165580000
H	-5.021106000	-4.982695000	-0.716835000
C	-4.839892000	-2.476235000	-1.884428000
C	-2.669391000	-2.575841000	1.248376000
C	-2.846107000	-3.903277000	1.676425000
H	-2.331530000	-4.255441000	2.570346000
C	-6.337975000	-0.442245000	-2.251904000
H	-7.047222000	-1.084995000	-2.775974000
C	-4.473826000	1.205083000	-0.938170000
C	-2.918060000	-1.829741000	4.737766000
H	-3.255875000	-2.813444000	4.382402000
H	-3.649827000	-1.479129000	5.481769000
H	-1.957676000	-1.954592000	5.253794000
C	-6.574701000	0.938048000	-2.166613000
C	-2.844130000	-0.817627000	3.579474000
H	-2.418625000	0.124035000	3.960793000
C	-4.257326000	-0.538227000	3.031458000
H	-4.228699000	0.091154000	2.133383000
H	-4.867524000	-0.034126000	3.795516000
H	-4.755229000	-1.478310000	2.759375000
C	-0.300895000	-2.214361000	2.979919000
H	-0.773711000	-2.894372000	3.705202000
C	-3.046520000	3.693704000	-1.439666000
H	-3.979613000	4.252773000	-1.252615000
C	-3.847722000	3.233515000	1.278580000
H	-3.777855000	4.283111000	0.952348000
C	-2.933839000	3.063885000	2.507837000
H	-2.950330000	2.029524000	2.872230000
H	-3.271680000	3.720555000	3.324511000
H	-1.890298000	3.312469000	2.274105000
C	0.535650000	-3.057682000	2.001957000
H	-0.077820000	-3.801278000	1.478175000
H	1.318497000	-3.592965000	2.560547000
H	1.017261000	-2.424721000	1.249761000
C	0.578972000	-1.206234000	3.748391000
H	1.055973000	-0.504812000	3.052007000
H	1.370556000	-1.740646000	4.294838000
H	0.002594000	-0.623490000	4.481417000
C	-5.321359000	2.948445000	1.620573000
H	-5.992084000	3.183704000	0.785885000
H	-5.621115000	3.567400000	2.480316000
H	-5.482248000	1.897748000	1.889080000
C	-3.010755000	3.316591000	-2.931578000
H	-2.071457000	2.819917000	-3.195869000
H	-3.095946000	4.237662000	-3.529132000
H	-3.835027000	2.650409000	-3.209904000
C	-1.857739000	4.610578000	-1.093319000
H	-1.866638000	4.940062000	-0.045327000
H	-1.885137000	5.511020000	-1.725303000
H	-0.908657000	4.092483000	-1.281247000
H	-3.821515000	-5.803346000	1.313765000
H	-4.134146000	-2.572848000	-2.731974000
H	-5.729662000	-3.065894000	-2.146460000
H	-7.471116000	1.373861000	-2.605179000
H	0.146300000	-0.953920000	-0.184355000
N	-1.137254000	0.872240000	-2.227276000
N	-0.106215000	0.996226000	-1.649781000

$TS_{2m'H}$(closed-shell singlet)

Ti	-1.328594000	0.239835000	-0.582237000
P	-2.706758000	2.569580000	-0.136732000
P	-2.732313000	-1.413292000	-2.049137000
N	-2.917323000	-0.228599000	0.681579000
C	-3.569682000	-1.470429000	0.601671000
C	-4.321199000	-3.398129000	-0.723099000
H	-4.354063000	-3.932668000	-1.673227000
C	-4.124504000	2.401445000	3.778570000
C	-3.320941000	0.622542000	1.727338000
C	-4.195937000	-2.050026000	1.741795000
C	-3.889403000	0.124178000	2.926346000
C	-4.288928000	1.016454000	3.927825000
H	-4.720298000	0.617465000	4.847466000
C	-3.994902000	-1.377636000	3.085792000
C	-3.206198000	2.031584000	1.547575000
C	-3.589393000	2.901458000	2.584871000
H	-3.481145000	3.977995000	2.454017000
C	-4.900293000	-3.250988000	1.615367000
H	-5.381462000	-3.672097000	2.499929000
C	-3.636648000	-2.170461000	-0.644049000
C	-4.881792000	4.517778000	-0.433953000
H	-5.024252000	4.539242000	0.655415000
H	-5.861057000	4.710755000	-0.898433000
H	-4.214488000	5.341437000	-0.717171000
C	-4.969893000	-3.937276000	0.392547000
C	-4.360760000	3.145268000	-0.898779000
H	-4.152803000	3.200254000	-1.979150000
C	-5.431501000	2.063056000	-0.655549000
H	-5.055436000	1.056933000	-0.876422000
H	-6.312335000	2.254114000	-1.286218000
H	-5.752228000	2.071036000	0.394309000
C	-1.757686000	4.182208000	0.093870000
H	-2.480846000	4.914964000	0.484165000
C	-1.890180000	-2.859781000	-2.929945000
H	-2.709221000	-3.459930000	-3.361857000
C	-3.987560000	-0.932937000	-3.413816000
H	-3.767419000	-1.631730000	-4.235933000
C	-3.694950000	0.495744000	-3.914252000
H	-3.877460000	1.234698000	-3.123816000
H	-4.346749000	0.740311000	-4.766692000
H	-2.651333000	0.606653000	-4.238738000
C	-0.596984000	4.076931000	1.103230000
H	-0.946494000	3.755648000	2.092562000
H	-0.128185000	5.067596000	1.209416000
H	0.157734000	3.362852000	0.757488000
C	-1.258729000	4.664421000	-1.285808000
H	-0.545958000	3.945274000	-1.709249000
H	-0.747831000	5.632992000	-1.180213000
H	-2.083391000	4.799437000	-2.001231000
C	-5.465047000	-1.117918000	-3.025790000
H	-5.693074000	-2.157747000	-2.763776000
H	-6.101729000	-0.832022000	-3.876951000
H	-5.744854000	-0.492128000	-2.170440000
C	-1.065723000	-3.748284000	-1.985901000
H	-0.254327000	-3.165983000	-1.531794000
H	-0.621401000	-4.576869000	-2.558471000
H	-1.680808000	-4.175226000	-1.184445000
C	-1.008859000	-2.317898000	-4.074559000

H	-1.577131000	-1.715396000	-4.796932000
H	-0.558306000	-3.157593000	-4.624451000
H	-0.201264000	-1.695810000	-3.667163000
H	-4.419288000	3.080404000	4.577371000
H	-3.061050000	-1.759897000	3.538456000
H	-4.805625000	-1.642145000	3.780294000
H	-5.511055000	-4.879103000	0.316950000
H	-0.135622000	-1.002741000	-1.236019000
Ti	1.328107000	-0.040252000	-0.440467000
P	2.020844000	-2.098659000	1.360237000
P	3.448921000	0.113260000	-2.045900000
N	2.790773000	0.634817000	0.810118000
C	3.870197000	1.419894000	0.376001000
C	5.541529000	1.972904000	-1.313608000
H	5.954695000	1.846244000	-2.313948000
C	2.362564000	0.014667000	4.961236000
C	2.678960000	0.440813000	2.199857000
C	4.438531000	2.394676000	1.239739000
C	3.112194000	1.424995000	3.117685000
C	2.949759000	1.198295000	4.490121000
H	3.274722000	1.962998000	5.197528000
C	3.707561000	2.693008000	2.537645000
C	2.175430000	-0.803019000	2.670144000
C	1.993433000	-0.987826000	4.051395000
H	1.582910000	-1.924355000	4.428068000
C	5.576326000	3.096590000	0.830718000
H	6.012290000	3.837659000	1.502989000
C	4.414926000	1.221968000	-0.927361000
C	3.916801000	-3.712567000	2.900164000
H	3.818509000	-3.021137000	3.748299000
H	4.933167000	-4.134739000	2.931373000
H	3.212186000	-4.541678000	3.042979000
C	6.140070000	2.887077000	-0.437749000
C	3.712314000	-2.973037000	1.563969000
H	3.734495000	-3.710537000	0.745489000
C	4.861541000	-1.969593000	1.349865000
H	4.729194000	-1.373603000	0.439905000
H	5.819212000	-2.507212000	1.279553000
H	4.925955000	-1.270395000	2.193990000
C	0.861700000	-3.389626000	2.099618000
H	1.236643000	-3.616193000	3.109731000
C	3.366284000	1.091510000	-3.679101000
H	4.367923000	0.961403000	-4.125646000
C	4.576172000	-1.303479000	-2.692269000
H	4.489066000	-1.206687000	-3.786058000
C	3.990845000	-2.676993000	-2.311903000
H	4.041517000	-2.848867000	-1.230613000
H	4.555405000	-3.480767000	-2.809881000
H	2.937042000	-2.759841000	-2.611123000
C	-0.578105000	-2.865308000	2.222797000
H	-0.622782000	-1.942475000	2.813912000
H	-1.207528000	-3.627323000	2.708589000
H	-1.002489000	-2.645525000	1.236884000
C	0.905490000	-4.689934000	1.269158000
H	0.587995000	-4.507510000	0.234752000
H	0.218907000	-5.431052000	1.704889000
H	1.907630000	-5.138363000	1.243579000
C	6.069549000	-1.199330000	-2.334789000
H	6.526108000	-0.289587000	-2.743842000
H	6.610291000	-2.061749000	-2.754862000
H	6.231212000	-1.194300000	-1.249922000
C	3.088032000	2.600783000	-3.555029000
H	2.091023000	2.772725000	-3.138066000
H	3.142984000	3.053329000	-4.558188000
H	3.823943000	3.102809000	-2.915766000
C	2.325433000	0.422360000	-4.601983000
H	2.517284000	-0.651665000	-4.743443000
H	2.344413000	0.897200000	-5.594936000
H	1.322720000	0.541120000	-4.173585000
H	2.218657000	-0.137642000	6.030148000
H	2.892275000	3.410813000	2.324678000
H	4.373984000	3.183085000	3.261893000
H	7.021067000	3.447690000	-0.747235000
H	-0.169211000	-0.420420000	0.699304000
N	0.892979000	1.403542000	-1.684537000
N	0.090724000	1.474614000	-0.659118000

H(closed-shell singlet)

Ti	1.271884000	0.266527000	-0.581428000
Ti	-1.262902000	0.232314000	0.043825000
P	2.374217000	2.519172000	0.007006000
P	-1.480434000	-0.986273000	2.377091000
P	-3.280459000	1.963049000	-0.439691000
P	2.235270000	-1.563433000	-2.162903000
N	-2.966528000	-0.979919000	-0.122349000
N	3.154831000	-0.287912000	0.338014000
N	-0.389742000	0.130533000	-1.640540000
N	-0.193471000	1.455809000	-1.225063000
C	-3.029831000	-2.249897000	0.494751000
C	3.716034000	1.984362000	1.119738000
C	4.615324000	-2.154840000	1.108162000
C	-2.450779000	-3.702880000	2.380532000
H	-1.935511000	-3.856928000	3.328538000
C	3.986009000	-3.608907000	-1.202038000
H	3.718943000	-4.183724000	-2.088658000
C	-4.055972000	-0.655708000	-0.954411000
C	3.722517000	-1.577327000	0.164032000
C	3.883927000	0.568695000	1.203403000
C	-3.112129000	3.235824000	-1.825462000
H	-4.115285000	3.664640000	-1.979616000
C	5.608080000	0.958422000	2.901042000
H	6.324797000	0.543004000	3.611794000
C	3.418618000	-2.337862000	-1.006136000
C	-2.371737000	-2.454320000	1.739723000
C	-4.405679000	0.709974000	-1.171239000
C	-3.190720000	-4.751761000	1.819141000
C	-4.374221000	-3.098879000	-1.441763000
C	-4.845396000	-1.666665000	-1.569191000
C	-3.761089000	-3.321847000	-0.077365000
C	-6.328083000	0.025552000	-2.517390000
C	2.594666000	0.037001000	-4.504615000
H	1.794587000	-0.416513000	-5.102569000
H	3.314452000	0.493096000	-5.200822000
H	2.142558000	0.837188000	-3.904229000
C	1.326650000	3.795941000	0.935570000
H	0.382339000	3.762781000	0.372710000
C	5.192313000	-3.408150000	0.869313000
H	5.878736000	-3.815433000	1.613773000
C	3.242892000	3.508510000	-1.348168000
H	3.697259000	4.386992000	-0.863547000
C	-5.974591000	-1.316747000	-2.315089000
H	-6.572592000	-2.110296000	-2.766436000
C	4.815844000	0.074835000	2.158870000
C	1.159247000	-2.979804000	-2.778724000
H	1.830862000	-3.718454000	-3.245515000
C	4.884948000	-4.150669000	-0.276659000
C	-3.844016000	-4.546635000	0.595949000
H	-4.414941000	-5.358246000	0.141684000
C	1.035655000	3.327940000	2.375766000
H	0.616585000	2.315138000	2.386737000
H	0.308025000	4.010293000	2.841301000
H	1.947843000	3.332770000	2.987186000
C	-4.074546000	-0.230578000	3.177344000
H	-4.087116000	0.227820000	2.181483000
H	-4.707598000	0.367620000	3.849591000
H	-4.520064000	-1.229801000	3.084071000
C	-5.527287000	1.027906000	-1.960403000
H	-5.775027000	2.072818000	-2.145658000

C	4.868448000	-1.414259000	2.398640000
C	-4.316354000	2.827274000	0.905528000
H	-4.863143000	1.988436000	1.359007000
C	2.229879000	3.977993000	-2.412014000
H	1.717425000	3.122536000	-2.870324000
H	2.750891000	4.539407000	-3.202398000
H	1.454579000	4.630265000	-1.989425000
C	4.522114000	2.847481000	1.882210000
H	4.397780000	3.924740000	1.777707000
C	-0.035462000	-1.677891000	3.370043000
H	-0.489361000	-2.270965000	4.179247000
C	-2.646865000	2.576840000	-3.140335000
H	-1.660342000	2.118656000	-3.005020000
H	-2.574487000	3.351056000	-3.920190000
H	-3.351073000	1.810043000	-3.484746000
C	3.313299000	-1.009402000	-3.624709000
H	4.145092000	-0.505659000	-3.107027000
C	0.140055000	-2.490974000	-3.829656000
H	-0.449930000	-1.653018000	-3.435997000
H	-0.544296000	-3.315718000	-4.080444000
H	0.626184000	-2.172433000	-4.760840000
C	3.902469000	-2.152147000	-4.471276000
H	4.474686000	-2.858759000	-3.857199000
H	4.584897000	-1.738116000	-5.229118000
H	3.116342000	-2.706137000	-5.002993000
C	5.486696000	2.347132000	2.763610000
C	1.846961000	5.248008000	0.939553000
H	2.786781000	5.343627000	1.499866000
H	1.105436000	5.891927000	1.436585000
H	2.006168000	5.648518000	-0.069026000
C	0.881938000	-2.607704000	2.555243000
H	0.323458000	-3.431400000	2.093830000
H	1.640560000	-3.040995000	3.225792000
H	1.394402000	-2.055646000	1.760495000
C	-2.141830000	4.363527000	-1.422138000
H	-2.457483000	4.890305000	-0.511253000
H	-2.083419000	5.106313000	-2.232357000
H	-1.141371000	3.942742000	-1.265462000
C	-2.644091000	-0.330792000	3.743269000
H	-2.275144000	0.686908000	3.948710000
C	0.770582000	-0.524144000	4.002141000
H	1.253783000	0.077704000	3.222630000
H	1.556964000	-0.933155000	4.654222000
H	0.143964000	0.141253000	4.613118000
C	-5.355441000	3.845941000	0.401889000
H	-4.878651000	4.721736000	-0.058883000
H	-5.956812000	4.206209000	1.250413000
H	-6.044997000	3.401044000	-0.326595000
C	4.373747000	2.674629000	-1.980824000
H	5.116360000	2.368948000	-1.233621000
H	4.883442000	3.266827000	-2.755636000
H	3.977849000	1.768538000	-2.458321000
C	0.436290000	-3.650549000	-1.592563000
H	1.142987000	-4.033250000	-0.845652000
H	-0.162132000	-4.495831000	-1.965014000
H	-0.236142000	-2.940832000	-1.096022000
C	-2.658235000	-1.127638000	5.061336000
H	-2.943408000	-2.174587000	4.885772000
H	-3.405580000	-0.692702000	5.742795000
H	-1.691036000	-1.110737000	5.579347000
C	-3.404521000	3.439251000	1.990187000
H	-2.687140000	2.700862000	2.372521000
H	-4.012233000	3.798590000	2.834383000
H	-2.832708000	4.294433000	1.604893000
H	0.172459000	-1.034868000	0.264645000
H	0.318575000	0.722838000	0.954566000
H	-7.202014000	0.283662000	-3.113657000
H	-3.608982000	-3.294313000	-2.217812000
H	-5.196447000	-3.804386000	-1.628495000
H	-3.254126000	-5.714432000	2.324408000
H	4.090020000	-1.689853000	3.136483000
H	5.830756000	-1.710423000	2.841091000
H	6.114300000	3.021364000	3.344406000
H	5.327376000	-5.132211000	-0.439839000

TS_{H2m}(closed-shell singlet)

Ti	1.270973000	0.289875000	-0.444999000
Ti	-1.298611000	0.293030000	0.140496000
P	2.669391000	2.417629000	0.138066000
P	-1.651189000	-1.215998000	2.286176000
P	-3.127793000	2.180571000	-0.238017000
P	2.076151000	-1.448544000	-2.216556000
N	-3.056940000	-0.812192000	-0.233153000
N	3.114743000	-0.473300000	0.372760000
N	-0.449362000	0.394022000	-1.539471000
N	0.229477000	1.523388000	-1.529190000
C	-3.233749000	-2.131313000	0.236666000
C	4.001091000	1.690005000	1.150589000
C	4.367185000	-2.523546000	1.004877000
C	-2.798957000	-3.833965000	1.947633000
H	-2.311912000	-4.133740000	2.875512000
C	3.528183000	-3.766816000	-1.363673000
H	3.190931000	-4.255365000	-2.277619000
C	-4.107311000	-0.303608000	-1.020980000
C	3.524566000	-1.802956000	0.114786000
C	3.989711000	0.264968000	1.204782000
C	-2.866009000	3.603535000	-1.451952000
H	-3.836176000	4.119034000	-1.533883000
C	5.839731000	0.379808000	2.803451000
H	6.532272000	-0.140601000	3.467511000
C	3.121016000	-2.447953000	-1.092965000
C	-2.614018000	-2.529687000	1.454927000
C	-4.342000000	1.102830000	-1.091110000
C	-3.609795000	-4.749220000	1.265539000
C	-4.621930000	-2.640929000	-1.784092000
C	-4.975004000	-1.170180000	-1.743903000
C	-4.043358000	-3.069321000	-0.454620000
C	-6.309388000	0.732710000	-2.494261000
C	2.696690000	0.236810000	-4.441183000
H	1.950183000	-0.130557000	-5.157009000
H	3.502906000	0.712169000	-5.019734000
H	2.215265000	1.001805000	-3.817945000
C	1.798494000	3.696893000	1.240767000
H	0.821665000	3.802860000	0.745335000
C	4.786095000	-3.821029000	0.690338000
H	5.437021000	-4.344818000	1.392593000
C	3.558073000	3.451794000	-1.167317000
H	4.098162000	4.247264000	-0.629711000
C	-6.066136000	-0.648091000	-2.443687000
H	-6.722131000	-1.335256000	-2.980762000
C	4.894131000	-0.373280000	2.099612000
C	0.889084000	-2.691984000	-2.990454000
H	1.502761000	-3.440900000	-3.516682000
C	4.365854000	-4.460370000	-0.483229000
C	-4.230713000	-4.352099000	0.072180000
H	-4.858312000	-5.057845000	-0.474613000
C	1.552178000	3.117139000	2.648679000
H	1.057670000	2.139838000	2.595969000
H	0.904087000	3.800639000	3.218629000
H	2.495332000	3.001566000	3.199031000
C	-4.216013000	-0.416422000	3.142628000
H	-4.194203000	0.154598000	2.206717000
H	-4.827554000	0.131508000	3.874873000
H	-4.708977000	-1.374239000	2.930604000
C	-5.431244000	1.597420000	-1.833755000
H	-5.590769000	2.673480000	-1.900713000
C	4.741677000	-1.861476000	2.309435000
C	-4.072103000	2.938995000	1.230198000

H	-4.673281000	2.090472000	1.586164000
C	2.539725000	4.085989000	-2.136081000
H	1.935587000	3.311193000	-2.624506000
H	3.068922000	4.663831000	-2.909035000
H	1.847936000	4.767119000	-1.622143000
C	4.961125000	2.420508000	1.873678000
H	4.978739000	3.506816000	1.791345000
C	-0.252779000	-2.088651000	3.197948000
H	-0.736522000	-2.713084000	3.964798000
C	-2.456293000	3.087021000	-2.846081000
H	-1.485699000	2.579502000	-2.795129000
H	-2.366658000	3.945571000	-3.529578000
H	-3.199762000	2.396040000	-3.261065000
C	3.275774000	-0.911722000	-3.587083000
H	4.109572000	-0.506958000	-2.991888000
C	-0.051376000	-2.012898000	-4.008036000
H	-0.592273000	-1.181601000	-3.536950000
H	-0.787746000	-2.747839000	-4.367277000
H	0.488084000	-1.630490000	-4.883522000
C	3.820281000	-2.054089000	-4.462870000
H	4.287296000	-2.842362000	-3.859059000
H	4.584083000	-1.661694000	-5.151441000
H	3.026147000	-2.504663000	-5.074937000
C	5.899867000	1.775685000	2.686624000
C	2.451913000	5.089777000	1.342755000
H	3.430857000	5.044291000	1.838730000
H	1.809525000	5.744292000	1.951710000
H	2.582360000	5.572822000	0.366552000
C	0.592153000	-3.008174000	2.297790000
H	-0.022873000	-3.764875000	1.795567000
H	1.339077000	-3.528549000	2.916948000
H	1.118889000	-2.432127000	1.530113000
C	-1.816192000	4.598552000	-0.918662000
H	-2.099809000	5.036852000	0.047644000
H	-1.695997000	5.423784000	-1.636581000
H	-0.847565000	4.095187000	-0.809801000
C	-2.800029000	-0.652341000	3.705377000
H	-2.382550000	0.316201000	4.023743000
C	0.629513000	-1.036323000	3.902163000
H	1.124999000	-0.396555000	3.160825000
H	1.407489000	-1.538253000	4.496690000
H	0.052655000	-0.393301000	4.582488000
C	-5.040523000	4.083663000	0.879613000
H	-4.507122000	4.976539000	0.526305000
H	-5.607164000	4.372125000	1.777826000
H	-5.766124000	3.784257000	0.112625000
C	4.592792000	2.596197000	-1.921344000
H	5.339683000	2.172056000	-1.238674000
H	5.114967000	3.216711000	-2.665249000
H	4.104153000	1.770411000	-2.453096000
C	0.069516000	-3.402789000	-1.894516000
H	0.710746000	-3.932160000	-1.179175000
H	-0.603475000	-4.136927000	-2.363217000
H	-0.539418000	-2.680481000	-1.337637000
C	-2.869546000	-1.585284000	4.928944000
H	-3.200777000	-2.592648000	4.639632000
H	-3.604357000	-1.190537000	5.647405000
H	-1.909149000	-1.669610000	5.453111000
C	-3.101966000	3.339285000	2.361903000
H	-2.440382000	2.505908000	2.634949000
H	-3.670135000	3.635419000	3.256579000
H	-2.467788000	4.188393000	2.073829000
H	0.097855000	-0.956449000	0.339582000
H	0.215815000	0.961320000	0.980677000
H	-7.155571000	1.125861000	-3.055585000
H	-5.495763000	-3.251147000	-2.053336000
H	-3.866119000	-2.805478000	-2.576381000
H	-3.754547000	-5.755867000	1.654907000
H	4.683829000	-5.477807000	-0.706004000
H	5.658710000	-2.300805000	2.727802000
H	3.940934000	-2.040432000	3.053481000
H	6.645802000	2.347704000	3.236374000

2m(closed-shell singlet)

Ti	1.361310000	0.388066000	-0.559139000
Ti	-1.260766000	0.150182000	-0.025601000
P	2.950856000	2.326511000	0.207028000
P	-1.802965000	-1.263973000	2.163009000
P	-2.698869000	2.335965000	-0.082433000
P	1.747646000	-1.600628000	-2.139295000
N	-3.183327000	-0.586855000	-0.311538000
N	3.143231000	-0.651661000	0.250282000
N	-0.394064000	0.811112000	-1.508043000
N	0.680829000	1.336423000	-2.031279000
C	-3.581463000	-1.861120000	0.149407000
C	4.312754000	1.398648000	0.976563000
C	4.111050000	-2.845623000	0.937482000
C	-3.393835000	-3.655824000	1.802411000
H	-2.935215000	-4.066731000	2.702085000
C	2.869011000	-4.076734000	-1.251227000
H	2.383458000	-4.550711000	-2.104395000
C	-4.154086000	0.143329000	-1.019568000
C	3.313577000	-2.045352000	0.072341000
C	4.144673000	-0.020364000	1.017614000
C	-2.280063000	3.835877000	-1.155485000
H	-3.164360000	4.491399000	-1.111336000
C	6.151774000	-0.119658000	2.426997000
H	6.835804000	-0.720037000	3.029700000
C	2.700174000	-2.697316000	-1.039474000
C	-2.990924000	-2.394431000	1.330793000
C	-4.109142000	1.567776000	-0.996572000
C	-4.388301000	-4.386336000	1.137318000
C	-5.144129000	-2.023231000	-1.805748000
C	-5.202771000	-0.511207000	-1.717478000
C	-4.585268000	-2.603612000	-0.522194000
C	-6.157609000	1.648923000	-2.328799000
C	2.522134000	-0.156761000	-4.519509000
H	1.883906000	-0.614332000	-5.287405000
H	3.388017000	0.282363000	-5.037524000
H	1.953147000	0.646157000	-4.033556000
C	2.317984000	3.538457000	1.517431000
H	1.380280000	3.909278000	1.077393000
C	4.282156000	-4.212373000	0.689586000
H	4.903603000	-4.790829000	1.375603000
C	3.749353000	3.387007000	-1.127360000
H	4.520395000	3.997559000	-0.630453000
C	-6.197989000	0.246832000	-2.342612000
H	-7.003127000	-0.268672000	-2.868841000
C	5.046847000	-0.750731000	1.849013000
C	0.402735000	-2.667187000	-2.913971000
H	0.914483000	-3.443944000	-3.505164000
C	3.660279000	-4.847242000	-0.392706000
C	-4.982638000	-3.845774000	-0.012491000
H	-5.759116000	-4.406062000	-0.536151000
C	1.966553000	2.768133000	2.806408000
H	1.273015000	1.943582000	2.598136000
H	1.487881000	3.451207000	3.524293000
H	2.871249000	2.358225000	3.275344000
C	-4.255146000	-0.286343000	3.189563000
H	-4.274553000	0.247455000	2.231983000
H	-4.759379000	0.332994000	3.946248000
H	-4.833566000	-1.210564000	3.061624000
C	-5.105515000	2.298207000	-1.670908000
H	-5.064122000	3.387011000	-1.680534000
C	4.718713000	-2.191724000	2.153326000
C	-3.505189000	3.077236000	1.476421000
H	-4.151966000	2.252119000	1.805646000
C	2.713898000	4.309576000	-1.799209000

H	1.912044000	3.715990000	-2.257285000
H	3.202363000	4.902359000	-2.587248000
H	2.260713000	5.011727000	-1.086329000
C	5.434643000	2.007345000	1.571052000
H	5.569908000	3.083723000	1.474035000
C	-0.507862000	-2.366435000	2.970737000
H	-1.018185000	-2.947635000	3.753708000
C	-2.023601000	3.466351000	-2.630842000
H	-1.118710000	2.858221000	-2.736194000
H	-1.886120000	4.395104000	-3.206456000
H	-2.865719000	2.917021000	-3.068164000
C	3.013355000	-1.212238000	-3.505608000
H	3.821764000	-0.761809000	-2.906725000
C	-0.503133000	-1.839330000	-3.851516000
H	-0.964084000	-1.006036000	-3.305489000
H	-1.304921000	-2.485658000	-4.239753000
H	0.041358000	-1.429896000	-4.709465000
C	3.581403000	-2.451864000	-4.221485000
H	3.995996000	-3.181148000	-3.515028000
H	4.388058000	-2.143453000	-4.903768000
H	2.812048000	-2.949529000	-4.829469000
C	6.383080000	1.254421000	2.268754000
C	3.221069000	4.747845000	1.829250000
H	4.141699000	4.437732000	2.339569000
H	2.685914000	5.430843000	2.506274000
H	3.494660000	5.318539000	0.932355000
C	0.135779000	-3.351456000	1.978745000
H	-0.608439000	-4.021391000	1.530326000
H	0.878806000	-3.967845000	2.506844000
H	0.651049000	-2.816281000	1.173333000
C	-1.074101000	4.603454000	-0.579779000
H	-1.254775000	4.970367000	0.438966000
H	-0.852660000	5.474306000	-1.215087000
H	-0.188564000	3.956833000	-0.568490000
C	-2.818102000	-0.609693000	3.647775000
H	-2.315230000	0.330209000	3.920611000
C	0.562450000	-1.468584000	3.627924000
H	1.084202000	-0.879400000	2.862565000
H	1.304052000	-2.091816000	4.149972000
H	0.132045000	-0.773455000	4.363179000
C	-4.395207000	4.314610000	1.261172000
H	-3.807818000	5.189268000	0.948582000
H	-4.895934000	4.577190000	2.205576000
H	-5.175891000	4.131646000	0.511853000
C	4.438151000	2.478229000	-2.164509000
H	5.174358000	1.813577000	-1.694193000
H	4.958627000	3.095780000	-2.911743000
H	3.696536000	1.864470000	-2.691833000
C	-0.450429000	-3.354939000	-1.830440000
H	0.149303000	-3.976977000	-1.156822000
H	-1.206808000	-3.992406000	-2.312298000
H	-0.980593000	-2.609721000	-1.222576000
C	-2.862617000	-1.523303000	4.887146000
H	-3.295696000	-2.503605000	4.642511000
H	-3.504587000	-1.063256000	5.654127000
H	-1.873668000	-1.680533000	5.335619000
C	-2.455782000	3.318353000	2.582585000
H	-1.789611000	2.453122000	2.696314000
H	-2.959993000	3.504255000	3.543018000
H	-1.831099000	4.195242000	2.364300000
H	0.235763000	-0.888008000	0.217891000
H	0.186605000	0.976961000	0.885506000
H	-6.930544000	2.227318000	-2.832754000
H	-6.133879000	-2.444727000	-2.032272000
H	-4.482453000	-2.306555000	-2.647331000
H	-4.697320000	-5.361941000	1.509807000
H	3.791008000	-5.914657000	-0.563630000
H	5.610352000	-2.738907000	2.492513000
H	3.995365000	-2.226861000	2.991791000
H	7.258058000	1.728579000	2.710303000

2m(triplet)

Ti	1.306326000	0.385604000	-0.528226000
Ti	-1.245217000	0.336365000	0.146046000
P	2.836161000	2.441801000	0.045183000
P	-1.734236000	-1.176228000	2.289247000
P	-3.101862000	2.228226000	-0.115554000
P	1.981357000	-1.537401000	-2.145725000
N	-2.970113000	-0.756658000	-0.330783000
N	3.043889000	-0.514003000	0.421304000
N	-0.428673000	1.039744000	-1.440174000
N	0.557267000	1.402540000	-2.104409000
C	-3.166123000	-2.079997000	0.108462000
C	4.067220000	1.622377000	1.109191000
C	4.157605000	-2.606373000	1.153398000
C	-2.802583000	-3.810890000	1.802770000
H	-2.359344000	-4.130074000	2.746186000
C	3.279448000	-3.892822000	-1.175998000
H	2.928862000	-4.394754000	-2.077777000
C	-3.983887000	-0.220480000	-1.141325000
C	3.367306000	-1.872884000	0.224398000
C	3.946655000	0.203805000	1.230246000
C	-2.860205000	3.789164000	-1.158908000
H	-3.856662000	4.250465000	-1.244124000
C	5.797858000	0.260623000	2.837293000
H	6.446579000	-0.277823000	3.530574000
C	2.934322000	-2.545859000	-0.957363000
C	-2.601141000	-2.494986000	1.349362000
C	-4.213371000	1.189415000	-1.156810000
C	-3.576038000	-4.715112000	1.063161000
C	-4.476670000	-2.536728000	-1.977184000
C	-4.819408000	-1.061526000	-1.927457000
C	-3.947961000	-3.000365000	-0.635959000
C	-6.090616000	0.875911000	-2.693559000
C	2.722322000	-0.131123000	-4.532740000
H	2.032906000	-0.601671000	-5.246955000
H	3.562788000	0.277914000	-5.113591000
H	2.195147000	0.699220000	-4.046659000
C	2.051628000	3.822581000	1.093503000
H	1.112395000	4.031240000	0.558526000
C	4.509768000	-3.934431000	0.894268000
H	5.120840000	-4.465500000	1.626277000
C	3.825396000	3.360066000	-1.273924000
H	4.460458000	4.092614000	-0.750994000
C	-5.865707000	-0.508981000	-2.671197000
H	-6.499413000	-1.171884000	-3.262877000
C	4.801484000	-0.451429000	2.164901000
C	0.700426000	-2.691609000	-2.918208000
H	1.246038000	-3.363378000	-3.600125000
C	4.071503000	-4.595122000	-0.261841000
C	-4.151876000	-4.294970000	-0.145340000
H	-4.755891000	-4.991257000	-0.729745000
C	1.689826000	3.295404000	2.496974000
H	1.097344000	2.374830000	2.435789000
H	1.098769000	4.055030000	3.031109000
H	2.595463000	3.091007000	3.083405000
C	-4.402295000	-0.610313000	3.025832000
H	-4.386126000	-0.061723000	2.076656000
H	-5.083570000	-0.094864000	3.719067000
H	-4.811676000	-1.607778000	2.819621000
C	-5.253798000	1.713641000	-1.947693000
H	-5.415442000	2.790930000	-1.980122000
C	4.542102000	-1.913736000	2.438605000
C	-4.212772000	2.801054000	1.323772000
H	-4.756884000	1.879475000	1.572325000
C	2.876672000	4.098019000	-2.240873000
H	2.207714000	3.388410000	-2.744284000
H	3.462831000	4.628218000	-3.006587000

H	2.251812000	4.840268000	-1.725450000
C	5.078707000	2.312421000	1.805148000
H	5.180988000	3.388194000	1.667976000
C	-0.360728000	-2.035156000	3.246133000
H	-0.847171000	-2.714293000	3.962919000
C	-2.349930000	3.487775000	-2.582331000
H	-1.331564000	3.085639000	-2.569643000
H	-2.342728000	4.424526000	-3.160874000
H	-2.993852000	2.769667000	-3.103588000
C	3.252150000	-1.158695000	-3.509791000
H	4.046934000	-0.675118000	-2.920137000
C	-0.332009000	-1.881012000	-3.733188000
H	-0.897444000	-1.208532000	-3.075305000
H	-1.043697000	-2.573205000	-4.208430000
H	0.126739000	-1.276138000	-4.523978000
C	3.862886000	-2.383556000	-4.214729000
H	4.315116000	-3.082884000	-3.501312000
H	4.651570000	-2.051624000	-4.907274000
H	3.112763000	-2.923723000	-4.809977000
C	5.963403000	1.641721000	2.654269000
C	2.845496000	5.140253000	1.205803000
H	3.783394000	5.000737000	1.759088000
H	2.244082000	5.872570000	1.765607000
H	3.081734000	5.584204000	0.230983000
C	0.561304000	-2.865655000	2.337143000
H	0.006642000	-3.636874000	1.788832000
H	1.325354000	-3.364988000	2.952251000
H	1.067496000	-2.226881000	1.606415000
C	-1.925048000	4.788962000	-0.449155000
H	-2.318822000	5.119215000	0.520633000
H	-1.792655000	5.682302000	-1.077685000
H	-0.936020000	4.342246000	-0.283122000
C	-2.997277000	-0.725386000	3.651907000
H	-2.680947000	0.272076000	3.994184000
C	0.441140000	-0.973657000	4.029381000
H	0.930755000	-0.277895000	3.335529000
H	1.219850000	-1.462905000	4.633504000
H	-0.192624000	-0.389159000	4.712049000
C	-5.257012000	3.880544000	0.985937000
H	-4.787080000	4.844754000	0.747255000
H	-5.912684000	4.041894000	1.855048000
H	-5.892780000	3.583069000	0.142262000
C	4.738695000	2.379692000	-2.032466000
H	5.425645000	1.859337000	-1.353184000
H	5.335629000	2.927886000	-2.776825000
H	4.141614000	1.627649000	-2.564132000
C	-0.027122000	-3.542627000	-1.857690000
H	0.657895000	-4.193697000	-1.303141000
H	-0.776583000	-4.175370000	-2.356970000
H	-0.546583000	-2.902106000	-1.135202000
C	-3.045613000	-1.669326000	4.867936000
H	-3.286052000	-2.697310000	4.561992000
H	-3.839019000	-1.336826000	5.554954000
H	-2.105004000	-1.683786000	5.432740000
C	-3.367343000	3.193376000	2.554200000
H	-2.627860000	2.418242000	2.795091000
H	-4.020032000	3.333812000	3.429025000
H	-2.824068000	4.134242000	2.392744000
H	0.108976000	-0.961446000	-0.001714000
H	0.320310000	1.035195000	0.958695000
H	-6.898799000	1.294817000	-3.291235000
H	-5.345725000	-3.133686000	-2.288938000
H	-3.695374000	-2.695594000	-2.745632000
H	-3.729533000	-5.731627000	1.422607000
H	4.337813000	-5.635380000	-0.442696000
H	5.415408000	-2.393298000	2.903459000
H	3.709992000	-2.002648000	3.164114000
H	6.748041000	2.183185000	3.180370000

$TS_{DE'}$(open-shell singlet)

Ti	1.340470000	0.392722000	-0.438587000
P	1.489817000	-1.314804000	-2.325479000
P	2.850120000	2.387211000	0.360615000
N	3.181167000	-0.573385000	0.034236000
C	4.171236000	-0.001703000	0.873500000
C	5.236913000	1.991077000	1.858305000
H	5.250817000	3.072988000	1.997063000
C	4.068192000	-4.464836000	-1.505945000
C	3.467968000	-1.877802000	-0.447052000
C	5.156576000	-0.788077000	1.536205000
C	4.419951000	-2.729585000	0.177656000
C	4.722008000	-3.983821000	-0.365525000
H	5.466040000	-4.603682000	0.137885000
C	5.025891000	-2.290492000	1.488135000
C	2.793356000	-2.379714000	-1.602930000
C	3.091232000	-3.661561000	-2.102326000
H	2.549239000	-4.035147000	-2.970466000
C	6.173296000	-0.180407000	2.280824000
H	6.918630000	-0.818243000	2.759263000
C	4.217035000	1.410488000	1.082470000
C	2.446011000	-1.797780000	-5.050600000
H	3.179545000	-2.535771000	-4.699035000
H	2.852615000	-1.332360000	-5.961567000
H	1.526499000	-2.326194000	-5.333494000
C	6.235699000	1.209447000	2.445933000
C	2.199634000	-0.714200000	-3.985573000
H	1.437105000	-0.013955000	-4.363645000
C	3.492352000	0.078919000	-3.714476000
H	3.323677000	0.889557000	-2.993313000
H	3.869702000	0.526414000	-4.646106000
H	4.274088000	-0.574976000	-3.304610000
C	0.120379000	-2.501826000	-2.848980000
H	0.561455000	-3.183402000	-3.593092000
C	2.388973000	3.585524000	1.750096000
H	3.301006000	4.173954000	1.946193000
C	3.653035000	3.592694000	-0.887936000
H	3.835827000	4.519739000	-0.320194000
C	2.670633000	3.909176000	-2.034915000
H	2.477729000	3.016281000	-2.645962000
H	3.097277000	4.680394000	-2.694014000
H	1.703115000	4.271264000	-1.667087000
C	-0.401144000	-3.340370000	-1.668047000
H	0.399522000	-3.928245000	-1.202279000
H	-1.172197000	-4.037089000	-2.030708000
H	-0.848292000	-2.696945000	-0.901330000
C	-1.025313000	-1.714413000	-3.515104000
H	-1.470737000	-1.010574000	-2.799565000
H	-1.811899000	-2.410026000	-3.843414000
H	-0.690869000	-1.148080000	-4.395747000
C	5.002122000	3.091303000	-1.437067000
H	5.747846000	2.972238000	-0.643217000
H	5.388238000	3.815126000	-2.170815000
H	4.897910000	2.122798000	-1.942926000
C	1.996620000	2.846969000	3.042416000
H	1.086441000	2.253475000	2.894632000
H	1.798813000	3.582976000	3.836452000
H	2.796123000	2.179210000	3.385719000
C	1.272458000	4.547118000	1.298389000
H	1.576019000	5.164150000	0.442204000
H	1.018887000	5.228707000	2.124096000
H	0.367294000	3.990347000	1.024602000
H	4.302726000	-5.448453000	-1.909946000
H	4.370134000	-2.621461000	2.317280000
H	5.998513000	-2.776077000	1.655101000
H	7.030313000	1.666957000	3.033113000
H	-0.228661000	1.231406000	-1.055780000
H	0.021604000	1.391564000	1.094662000
Ti	-1.337323000	0.460507000	0.249338000

P	-1.359420000	-0.892743000	2.431993000
P	-3.055430000	2.196385000	-0.687287000
N	-3.139491000	-0.693976000	0.054215000
C	-4.194025000	-0.328097000	-0.815508000
C	-5.449776000	1.411031000	-2.027056000
H	-5.559467000	2.457910000	-2.314630000
C	-3.746733000	-4.296183000	2.263469000
C	-3.324511000	-1.910962000	0.751708000
C	-5.130427000	-1.278441000	-1.317449000
C	-4.226602000	-2.916344000	0.306117000
C	-4.441873000	-4.069806000	1.069152000
H	-5.149692000	-4.814735000	0.700730000
C	-4.872068000	-2.741092000	-1.047281000
C	-2.603862000	-2.154333000	1.960443000
C	-2.816937000	-3.340215000	2.687323000
H	-2.246418000	-3.518554000	3.598416000
C	-6.214534000	-0.866630000	-2.099235000
H	-6.919373000	-1.622841000	-2.450052000
C	-4.363366000	1.031338000	-1.218523000
C	-2.197693000	-0.930742000	5.245652000
H	-2.880534000	-1.772658000	5.067411000
H	-2.617482000	-0.332942000	6.069512000
H	-1.233844000	-1.330155000	5.587820000
C	-6.395610000	0.476091000	-2.458937000
C	-2.063962000	-0.053397000	3.988090000
H	-1.344799000	0.757117000	4.191070000
C	-3.415044000	0.589891000	3.626451000
H	-3.312732000	1.227143000	2.738748000
H	-3.781822000	1.206518000	4.461108000
H	-4.168888000	-0.179339000	3.408625000
C	0.073181000	-1.908109000	3.128157000
H	-0.324543000	-2.464817000	3.990934000
C	-2.669092000	3.118497000	-2.296075000
H	-3.616920000	3.579648000	-2.620352000
C	-3.944352000	3.563901000	0.306063000
H	-4.243463000	4.317326000	-0.441849000
C	-2.980927000	4.224424000	1.313041000
H	-2.640417000	3.494538000	2.059040000
H	-3.494059000	5.046398000	1.835692000
H	-2.087926000	4.635857000	0.826644000
C	0.619036000	-2.923996000	2.109066000
H	-0.159311000	-3.622609000	1.778216000
H	1.430340000	-3.507055000	2.572060000
H	1.020710000	-2.413874000	1.225643000
C	1.189263000	-0.968563000	3.623879000
H	1.588804000	-0.375366000	2.789425000
H	2.016618000	-1.558131000	4.047108000
H	0.838909000	-0.276097000	4.402082000
C	-5.215657000	3.062662000	1.018304000
H	-5.958960000	2.679650000	0.310326000
H	-5.667515000	3.893717000	1.581225000
H	-4.986546000	2.260242000	1.730553000
C	-2.190095000	2.149463000	-3.392381000
H	-1.254761000	1.661245000	-3.088465000
H	-2.005108000	2.706810000	-4.323856000
H	-2.937253000	1.373419000	-3.600271000
C	-1.632075000	4.233058000	-2.061576000
H	-1.999566000	5.006771000	-1.374620000
H	-1.391593000	4.724324000	-3.016812000
H	-0.706234000	3.809984000	-1.649278000
H	-3.914110000	-5.203589000	2.842035000
H	-4.191502000	-3.137914000	-1.826819000
H	-5.799848000	-3.327038000	-1.122742000
H	-7.241095000	0.779751000	-3.074443000
H	-0.834285000	1.781108000	1.410376000
H	0.011060000	-0.788317000	-0.015943000

$TS_{DE'}$(quintet)

Ti	1.310612000	0.241545000	-0.150657000
P	1.774282000	-1.376178000	-2.141304000
P	2.873740000	2.310445000	0.167868000
N	3.123123000	-0.651303000	0.373771000
C	4.114419000	0.010823000	1.129129000
C	5.218159000	2.086223000	1.815000000
H	5.273250000	3.175251000	1.796548000
C	4.061395000	-4.614311000	-0.836677000
C	3.430302000	-1.977535000	-0.003861000
C	5.047763000	-0.713378000	1.919404000
C	4.317043000	-2.782123000	0.757481000
C	4.631654000	-4.075575000	0.325624000
H	5.319886000	-4.676661000	0.922414000
C	4.843968000	-2.207486000	2.054131000
C	2.865355000	-2.514810000	-1.196858000
C	3.175336000	-3.830808000	-1.586312000
H	2.725586000	-4.244837000	-2.488708000
C	6.065692000	-0.034502000	2.597356000
H	6.778367000	-0.610728000	3.189990000
C	4.202918000	1.432837000	1.091458000
C	2.940842000	-1.968256000	-4.761878000
H	3.412646000	-2.879399000	-4.368350000
H	3.582798000	-1.588030000	-5.571378000
H	1.974745000	-2.239321000	-5.206442000
C	6.163358000	1.364008000	2.552318000
C	2.809503000	-0.895356000	-3.665599000
H	2.277705000	-0.024200000	-4.080303000
C	4.202453000	-0.439500000	-3.190350000
H	4.128523000	0.256329000	-2.345522000
H	4.740144000	0.058917000	-4.010468000
H	4.798043000	-1.301114000	-2.860458000
C	0.428030000	-2.487556000	-2.845238000
H	0.917672000	-3.210561000	-3.516293000
C	2.401877000	3.683896000	1.392635000
H	3.301942000	4.316071000	1.481490000
C	3.714826000	3.395884000	-1.175561000
H	3.692380000	4.420577000	-0.771035000
C	2.865026000	3.365613000	-2.462022000
H	2.838154000	2.354094000	-2.889308000
H	3.291609000	4.047123000	-3.214366000
H	1.826737000	3.667857000	-2.274148000
C	-0.292220000	-3.264221000	-1.727986000
H	0.400544000	-3.902826000	-1.165865000
H	-1.065987000	-3.909615000	-2.171857000
H	-0.769385000	-2.575255000	-1.020839000
C	-0.564689000	-1.637480000	-3.664209000
H	-1.048530000	-0.890998000	-3.021442000
H	-1.345819000	-2.282246000	-4.094721000
H	-0.074633000	-1.107931000	-4.493798000
C	5.181866000	3.032027000	-1.467792000
H	5.820136000	3.146717000	-0.584346000
H	5.569987000	3.691003000	-2.259913000
H	5.281550000	1.996496000	-1.815521000
C	2.035143000	3.142183000	2.784351000
H	1.137873000	2.514926000	2.720498000
H	1.817813000	3.984988000	3.458720000
H	2.849773000	2.553298000	3.223523000
C	1.248309000	4.535547000	0.831040000
H	1.481855000	4.966500000	-0.152601000
H	1.033765000	5.369407000	1.516933000
H	0.341765000	3.922804000	0.740989000
H	4.302977000	-5.628644000	-1.151205000
H	4.107237000	-2.397838000	2.858905000
H	5.774172000	-2.707745000	2.359656000
H	6.954066000	1.880812000	3.094351000
H	-0.195746000	0.964409000	-1.056564000
H	0.315969000	1.214309000	1.125339000
Ti	-1.310313000	0.605586000	0.438250000
P	-2.038050000	-0.495600000	2.631653000
P	-2.942788000	2.140189000	-0.876035000

N	-2.910528000	-0.768359000	-0.144807000
C	-3.772531000	-0.519806000	-1.221223000
C	-4.822113000	1.076105000	-2.756287000
H	-4.948337000	2.098076000	-3.113770000
C	-3.352790000	-4.400204000	1.989202000
C	-3.103870000	-1.969643000	0.550247000
C	-4.493432000	-1.566641000	-1.866902000
C	-3.742092000	-3.096636000	-0.038435000
C	-3.857725000	-4.287650000	0.685396000
H	-4.338172000	-5.146102000	0.213537000
C	-4.209346000	-2.997051000	-1.470878000
C	-2.651734000	-2.064794000	1.905265000
C	-2.755009000	-3.286038000	2.591996000
H	-2.391005000	-3.362243000	3.615907000
C	-5.371685000	-1.271137000	-2.913358000
H	-5.912458000	-2.087872000	-3.393948000
C	-3.946000000	0.823335000	-1.685237000
C	-3.833030000	-0.702155000	4.922972000
H	-4.065654000	-1.744064000	4.661149000
H	-4.719014000	-0.280844000	5.422384000
H	-3.012263000	-0.701298000	5.651461000
C	-5.546582000	0.045061000	-3.365158000
C	-3.511287000	0.122921000	3.663144000
H	-3.209977000	1.140398000	3.959208000
C	-4.752425000	0.226460000	2.758148000
H	-4.516576000	0.744934000	1.820877000
H	-5.553291000	0.777415000	3.273152000
H	-5.133029000	-0.772335000	2.503941000
C	-0.785989000	-1.001515000	3.945659000
H	-1.308092000	-1.682956000	4.636194000
C	-2.357306000	3.152260000	-2.378358000
H	-3.274120000	3.569033000	-2.829324000
C	-4.173308000	3.429085000	-0.149312000
H	-4.166773000	4.265114000	-0.867247000
C	-3.632121000	3.944183000	1.199208000
H	-3.580992000	3.132580000	1.937017000
H	-4.290005000	4.735022000	1.592236000
H	-2.617900000	4.353336000	1.104353000
C	0.418665000	-1.745858000	3.341224000
H	0.110194000	-2.631152000	2.771246000
H	1.089776000	-2.069921000	4.151928000
H	0.980099000	-1.093181000	2.661708000
C	-0.326286000	0.241058000	4.736214000
H	0.160414000	0.961551000	4.067734000
H	0.399621000	-0.057098000	5.507209000
H	-1.159671000	0.750377000	5.239254000
C	-5.625228000	2.935156000	-0.014881000
H	-6.060228000	2.657579000	-0.982032000
H	-6.242794000	3.735848000	0.420595000
H	-5.698225000	2.062197000	0.645082000
C	-1.626993000	2.302879000	-3.431928000
H	-0.729645000	1.843809000	-2.998702000
H	-1.323326000	2.945514000	-4.273215000
H	-2.267646000	1.504709000	-3.827200000
C	-1.466194000	4.319141000	-1.913802000
H	-1.967221000	4.970766000	-1.184759000
H	-1.183058000	4.940192000	-2.777319000
H	-0.549976000	3.930067000	-1.453807000
H	-3.446714000	-5.337429000	2.535963000
H	-3.422438000	-3.399528000	-2.136417000
H	-5.094600000	-3.629302000	-1.635367000
H	-6.233833000	0.261151000	-4.181990000
H	-1.144620000	1.872356000	1.756158000
H	-0.121997000	-0.850651000	0.449363000

E'(open-shell singlet)

Ti	1.393496000	0.431284000	-0.389100000
P	1.513326000	-1.213232000	-2.325200000
P	3.044629000	2.360263000	0.372387000
N	3.183812000	-0.622176000	0.085005000
C	4.214569000	-0.102515000	0.900506000
C	5.431197000	1.829931000	1.830355000
H	5.521907000	2.910674000	1.949300000
C	3.856361000	-4.542112000	-1.469962000
C	3.398079000	-1.936166000	-0.401795000
C	5.151884000	-0.944179000	1.567983000
C	4.288812000	-2.845059000	0.231072000
C	4.521547000	-4.112443000	-0.315160000
H	5.218757000	-4.780880000	0.193196000
C	4.906725000	-2.433792000	1.545898000
C	2.715910000	-2.380076000	-1.575613000
C	2.944398000	-3.674218000	-2.080103000
H	2.401294000	-4.006738000	-2.964191000
C	6.219186000	-0.395319000	2.284963000
H	6.925322000	-1.073364000	2.767658000
C	4.362525000	1.308227000	1.076855000
C	2.493030000	-1.703594000	-5.048274000
H	3.107662000	-2.545904000	-4.702440000
H	2.998997000	-1.260061000	-5.919740000
H	1.526938000	-2.094392000	-5.392623000
C	6.380630000	0.991225000	2.420075000
C	2.341508000	-0.641138000	-3.944609000
H	1.678796000	0.158944000	-4.313959000
C	3.710216000	-0.018737000	-3.608806000
H	3.622910000	0.740353000	-2.820483000
H	4.144257000	0.456963000	-4.501108000
H	4.409554000	-0.787098000	-3.252351000
C	0.107220000	-2.311859000	-2.942857000
H	0.539528000	-2.996157000	-3.689332000
C	2.639798000	3.541918000	1.794855000
H	3.570627000	4.097061000	1.998630000
C	3.861581000	3.564540000	-0.864476000
H	4.034819000	4.494239000	-0.298294000
C	2.883265000	3.869632000	-2.018628000
H	2.695122000	2.968722000	-2.619624000
H	3.309973000	4.635582000	-2.683791000
H	1.913666000	4.233446000	-1.655680000
C	-0.509147000	-3.151984000	-1.810026000
H	0.234587000	-3.808375000	-1.341475000
H	-1.313871000	-3.782008000	-2.219073000
H	-0.934797000	-2.506364000	-1.032940000
C	-0.963163000	-1.442230000	-3.631661000
H	-1.407578000	-0.742669000	-2.911147000
H	-1.768167000	-2.080863000	-4.025113000
H	-0.556319000	-0.860821000	-4.471372000
C	5.217045000	3.068265000	-1.401089000
H	5.952922000	2.938877000	-0.599620000
H	5.613102000	3.800410000	-2.121106000
H	5.117992000	2.106165000	-1.919330000
C	2.239301000	2.778228000	3.070135000
H	1.334178000	2.179361000	2.903819000
H	2.029311000	3.494196000	3.879120000
H	3.037766000	2.105055000	3.404631000
C	1.550057000	4.549569000	1.379228000
H	1.859223000	5.167540000	0.525565000
H	1.333159000	5.227703000	2.218139000
H	0.621108000	4.030797000	1.108307000
H	4.035198000	-5.535892000	-1.877913000
H	4.212972000	-2.695766000	2.368916000
H	5.835888000	-2.989877000	1.737874000
H	7.213844000	1.402992000	2.987320000
H	-0.168380000	1.461109000	-0.735013000
H	-0.308351000	1.656872000	1.473752000
Ti	-1.378832000	0.485845000	0.324700000
P	-1.527900000	-0.989858000	2.416759000
P	-3.069276000	2.298801000	-0.527534000
N	-3.149546000	-0.648882000	-0.048196000
C	-4.164156000	-0.217050000	-0.932715000

C	-5.374733000	1.609087000	-2.058585000
H	-5.480255000	2.675216000	-2.265531000
C	-3.860827000	-4.392064000	1.870265000
C	-3.370031000	-1.909400000	0.554499000
C	-5.066659000	-1.128715000	-1.554116000
C	-4.239857000	-2.881562000	-0.010977000
C	-4.489769000	-4.085814000	0.656588000
H	-5.170752000	-4.805779000	0.198895000
C	-4.811120000	-2.607075000	-1.381625000
C	-2.720190000	-2.230183000	1.784193000
C	-2.964850000	-3.464876000	2.413832000
H	-2.446017000	-3.704095000	3.341736000
C	-6.113263000	-0.660289000	-2.354287000
H	-6.793883000	-1.388234000	-2.799768000
C	-4.329120000	1.170915000	-1.224939000
C	-2.487155000	-1.223322000	5.185929000
H	-3.112394000	-2.089395000	4.929154000
H	-2.979852000	-0.694942000	6.016836000
H	-1.520261000	-1.588327000	5.556083000
C	-6.286058000	0.706731000	-2.614828000
C	-2.341562000	-0.272362000	3.984193000
H	-1.673487000	0.557866000	4.268163000
C	-3.708210000	0.323542000	3.597834000
H	-3.611709000	0.996184000	2.735634000
H	-4.131853000	0.890177000	4.440893000
H	-4.416164000	-0.471343000	3.325714000
C	-0.114406000	-2.025671000	3.123965000
H	-0.539526000	-2.627770000	3.941969000
C	-2.586116000	3.338348000	-2.036647000
H	-3.512937000	3.826190000	-2.382244000
C	-4.017506000	3.597429000	0.504871000
H	-4.243174000	4.419101000	-0.194984000
C	-3.125626000	4.148244000	1.636873000
H	-2.903939000	3.361600000	2.371100000
H	-3.644981000	4.966244000	2.159069000
H	-2.168055000	4.535736000	1.265788000
C	0.489020000	-2.983173000	2.080836000
H	-0.262744000	-3.678401000	1.687386000
H	1.292183000	-3.573690000	2.548420000
H	0.914266000	-2.425247000	1.238507000
C	0.966669000	-1.094524000	3.706969000
H	1.399314000	-0.471757000	2.911036000
H	1.778869000	-1.690438000	4.150079000
H	0.572299000	-0.430822000	4.489822000
C	-5.347542000	3.067665000	1.074020000
H	-6.040539000	2.761308000	0.282696000
H	-5.828651000	3.857772000	1.670662000
H	-5.185905000	2.202817000	1.729873000
C	-2.041057000	2.450029000	-3.169829000
H	-1.129716000	1.930773000	-2.843928000
H	-1.791471000	3.073718000	-4.042262000
H	-2.777191000	1.700001000	-3.484698000
C	-1.565001000	4.427656000	-1.658396000
H	-1.963179000	5.136427000	-0.920009000
H	-1.287486000	5.003647000	-2.554384000
H	-0.654616000	3.968964000	-1.249526000
H	-4.053331000	-5.338810000	2.373009000
H	-4.084614000	-2.939681000	-2.149169000
H	-5.728293000	-3.189374000	-1.552956000
H	-7.100881000	1.054875000	-3.247845000
H	-1.066639000	1.888802000	1.654664000
H	0.019040000	-0.716262000	0.063831000

E'(quintet)

Ti	1.418305000	0.475176000	-0.276538000
P	1.696961000	-0.952864000	-2.388229000
P	3.182859000	2.284853000	0.470909000
N	3.123826000	-0.683955000	0.187101000
C	4.162896000	-0.249445000	1.034151000
C	5.472687000	1.579960000	2.026987000
H	5.637448000	2.649281000	2.167484000
C	3.709607000	-4.511183000	-1.581406000
C	3.311985000	-1.967737000	-0.375204000
C	5.013966000	-1.168986000	1.711549000
C	4.107224000	-2.958479000	0.259454000
C	4.308691000	-4.200304000	-0.352853000
H	4.928701000	-4.941911000	0.153968000
C	4.662443000	-2.637152000	1.628144000
C	2.711856000	-2.280147000	-1.629861000
C	2.906571000	-3.549731000	-2.205811000
H	2.428810000	-3.788050000	-3.155796000
C	6.087917000	-0.706612000	2.477109000
H	6.730251000	-1.436070000	2.973625000
C	4.404047000	1.145662000	1.217505000
C	2.886758000	-1.280278000	-5.051597000
H	3.349132000	-2.229477000	-4.747328000
H	3.538913000	-0.823984000	-5.812297000
H	1.924092000	-1.499117000	-5.531405000
C	6.332498000	0.665921000	2.642124000
C	2.748123000	-0.325650000	-3.851786000
H	2.225436000	0.587206000	-4.183029000
C	4.137225000	0.075586000	-3.320745000
H	4.052810000	0.707655000	-2.427242000
H	4.697642000	0.625964000	-4.091357000
H	4.716618000	-0.815152000	-3.042769000
C	0.293001000	-1.875576000	-3.247748000
H	0.757941000	-2.526768000	-4.004121000
C	2.714456000	3.353893000	1.969581000
H	3.648454000	3.840136000	2.297321000
C	4.117066000	3.580389000	-0.581383000
H	4.255012000	4.455836000	0.073913000
C	3.230454000	3.994692000	-1.775191000
H	3.067269000	3.142068000	-2.449821000
H	3.717869000	4.795997000	-2.351118000
H	2.245193000	4.357971000	-1.453480000
C	-0.501881000	-2.755842000	-2.266448000
H	0.140953000	-3.494910000	-1.772631000
H	-1.286414000	-3.297974000	-2.816540000
H	-0.977992000	-2.146113000	-1.489846000
C	-0.630997000	-0.870606000	-3.963811000
H	-1.108343000	-0.203313000	-3.234100000
H	-1.427238000	-1.407487000	-4.500835000
H	-0.092135000	-0.251875000	-4.695711000
C	5.503403000	3.113538000	-1.061427000
H	6.172493000	2.879950000	-0.225756000
H	5.967139000	3.909538000	-1.663928000
H	5.430619000	2.217252000	-1.689667000
C	2.184715000	2.481548000	3.121867000
H	1.282330000	1.934523000	2.813141000
H	1.917969000	3.116161000	3.980939000
H	2.932066000	1.750235000	3.452447000
C	1.694325000	4.442843000	1.591695000
H	2.067904000	5.113432000	0.806006000
H	1.462684000	5.060700000	2.472634000
H	0.760695000	3.984503000	1.239804000
H	3.862036000	-5.486907000	-2.040641000
H	3.894817000	-2.866126000	2.393063000
H	5.532579000	-3.267240000	1.862211000
H	7.168117000	1.011248000	3.249119000
H	-0.025070000	1.699753000	0.113822000
H	-0.852039000	1.895752000	1.938806000
Ti	-1.453386000	0.510525000	0.558188000
P	-1.818788000	-1.236740000	2.381465000
P	-3.085074000	2.397884000	-0.286918000
N	-3.122059000	-0.593650000	-0.212376000
C	-4.037898000	-0.065581000	-1.146561000
C	-5.164214000	1.878939000	-2.158755000
H	-5.277009000	2.961670000	-2.234708000

C	-3.885582000	-4.593296000	1.068378000
C	-3.361643000	-1.929773000	0.181132000
C	-4.838466000	-0.897114000	-1.983567000
C	-4.124134000	-2.833758000	-0.609974000
C	-4.391645000	-4.128562000	-0.152721000
H	-4.987869000	-4.791624000	-0.782346000
C	-4.563742000	-2.381853000	-1.982100000
C	-2.844518000	-2.409528000	1.422986000
C	-3.100994000	-3.729527000	1.839304000
H	-2.680003000	-4.085114000	2.779410000
C	-5.799172000	-0.339933000	-2.832517000
H	-6.403051000	-1.010791000	-3.446402000
C	-4.209687000	1.346837000	-1.270770000
C	-3.151406000	-1.905614000	4.908099000
H	-3.703020000	-2.728003000	4.432773000
H	-3.773595000	-1.521133000	5.730944000
H	-2.233368000	-2.311843000	5.352208000
C	-5.979391000	1.047645000	-2.931218000
C	-2.872231000	-0.775694000	3.900737000
H	-2.281898000	0.008631000	4.404048000
C	-4.192310000	-0.147119000	3.415142000
H	-4.004575000	0.662668000	2.697407000
H	-4.756887000	0.261929000	4.266629000
H	-4.818782000	-0.897806000	2.914241000
C	-0.445914000	-2.295351000	3.132270000
H	-0.931725000	-3.038257000	3.783798000
C	-2.426704000	3.588227000	-1.608870000
H	-3.315307000	4.061063000	-2.058957000
C	-4.192619000	3.578414000	0.729225000
H	-4.356496000	4.459607000	0.087045000
C	-3.461585000	4.031312000	2.010791000
H	-3.340734000	3.186439000	2.702986000
H	-4.049104000	4.806895000	2.524845000
H	-2.463709000	4.440363000	1.805726000
C	0.357738000	-3.045192000	2.054566000
H	-0.284639000	-3.700964000	1.454083000
H	1.126883000	-3.666439000	2.538932000
H	0.854216000	-2.342524000	1.375093000
C	0.476341000	-1.412000000	3.996915000
H	0.961553000	-0.643112000	3.379334000
H	1.267072000	-2.026951000	4.452102000
H	-0.065639000	-0.908975000	4.810447000
C	-5.563652000	2.970629000	1.080929000
H	-6.146631000	2.723805000	0.186887000
H	-6.138370000	3.690864000	1.683136000
H	-5.452827000	2.052148000	1.671756000
C	-1.672143000	2.815062000	-2.704995000
H	-0.798658000	2.298594000	-2.280706000
H	-1.315374000	3.513433000	-3.477739000
H	-2.316006000	2.069562000	-3.187411000
C	-1.535499000	4.688150000	-1.004987000
H	-2.071622000	5.310339000	-0.276082000
H	-1.174202000	5.352756000	-1.804592000
H	-0.661587000	4.244410000	-0.511019000
H	-4.087587000	-5.609443000	1.403991000
H	-3.758597000	-2.600151000	-2.710497000
H	-5.445113000	-2.946333000	-2.320374000
H	-6.726364000	1.466432000	-3.603868000
H	-1.481730000	1.618430000	2.295583000
H	-0.060199000	-0.662159000	0.064628000

$TS_{EF'}$(closed-shell singlet)

Ti	-1.306958000	0.691565000	0.573332000
P	-1.358741000	-0.790989000	2.669742000
P	-2.808762000	2.147262000	-0.941976000
N	-2.954892000	-0.662703000	0.149692000
C	-3.834047000	-0.447779000	-0.945534000
C	-4.807497000	1.093083000	-2.618177000
H	-4.831388000	2.088954000	-3.063543000
C	-3.631603000	-4.240199000	2.440530000
C	-3.167727000	-1.868761000	0.875599000
C	-4.697056000	-1.452554000	-1.473533000
C	-4.012242000	-2.920717000	0.413608000
C	-4.249646000	-4.054586000	1.199900000
H	-4.917582000	-4.822586000	0.805223000
C	-4.576374000	-2.869984000	-0.981790000
C	-2.513064000	-2.089950000	2.127013000
C	-2.744625000	-3.254498000	2.880214000
H	-2.213516000	-3.391988000	3.821737000
C	-5.600949000	-1.162220000	-2.502493000
H	-6.246199000	-1.965948000	-2.862050000
C	-3.907411000	0.835300000	-1.568758000
C	-2.095240000	-0.812799000	5.504519000
H	-2.573443000	-1.798162000	5.418804000
H	-2.618830000	-0.263937000	6.302282000
H	-1.056930000	-0.955350000	5.829317000
C	-5.675080000	0.105806000	-3.089320000
C	-2.209150000	-0.018224000	4.189638000
H	-1.698786000	0.948930000	4.316278000
C	-3.693199000	0.254710000	3.867565000
H	-3.816281000	0.787538000	2.918142000
H	-4.138795000	0.866475000	4.666405000
H	-4.253049000	-0.687692000	3.802467000
C	0.111877000	-1.720145000	3.389043000
H	-0.278811000	-2.309066000	4.233592000
C	-2.108084000	3.033306000	-2.461392000
H	-2.926353000	3.673527000	-2.833111000
C	-4.122569000	3.386695000	-0.331834000
H	-4.819486000	3.465121000	-1.182868000
C	-3.592130000	4.796436000	-0.008775000
H	-2.822323000	4.772252000	0.773178000
H	-4.423142000	5.417677000	0.359141000
H	-3.176189000	5.295070000	-0.893167000
C	0.725728000	-2.690710000	2.365017000
H	-0.012439000	-3.414082000	1.997794000
H	1.547721000	-3.249014000	2.839046000
H	1.132888000	-2.144135000	1.506021000
C	1.166177000	-0.728922000	3.920718000
H	1.574685000	-0.127080000	3.099966000
H	1.994227000	-1.281888000	4.388875000
H	0.753004000	-0.042346000	4.672940000
C	-4.892852000	2.798702000	0.865057000
H	-5.277222000	1.794066000	0.646484000
H	-5.747909000	3.446952000	1.109109000
H	-4.251615000	2.739795000	1.753995000
C	-1.679767000	2.063411000	-3.578085000
H	-0.876493000	1.409292000	-3.216479000
H	-1.292871000	2.645288000	-4.428922000
H	-2.509184000	1.441170000	-3.933566000
C	-0.906234000	3.917064000	-2.063187000
H	-1.137216000	4.616672000	-1.251158000
H	-0.580504000	4.504238000	-2.935678000
H	-0.073224000	3.279652000	-1.741909000
H	-3.817232000	-5.134754000	3.032850000
H	-3.907722000	-3.434400000	-1.660955000
H	-5.549458000	-3.382440000	-1.028238000
H	-6.381500000	0.313601000	-3.891398000
H	0.467973000	0.924473000	1.139356000
H	-0.395036000	1.071242000	-0.951553000
Ti	1.268889000	0.373366000	-0.451771000
P	1.251920000	-1.353238000	-2.355984000
P	2.900769000	2.267695000	0.266980000
N	2.996609000	-0.719623000	-0.015653000
C	3.985506000	-0.231691000	0.886788000
C	5.118696000	1.665183000	1.958110000
H	5.208951000	2.740217000	2.111317000
C	3.854217000	-4.534845000	-1.750433000
C	3.255264000	-2.013983000	-0.553150000

C	4.891725000	-1.093643000	1.561786000
C	4.163380000	-2.920691000	0.057204000
C	4.470094000	-4.141057000	-0.557801000
H	5.187913000	-4.802939000	-0.070421000
C	4.718832000	-2.584486000	1.418594000
C	2.590474000	-2.442604000	-1.738900000
C	2.892949000	-3.689262000	-2.314443000
H	2.362789000	-4.006711000	-3.211368000
C	5.898705000	-0.568601000	2.380672000
H	6.584052000	-1.261187000	2.872013000
C	4.109385000	1.168894000	1.114350000
C	1.694958000	-1.809956000	-5.210656000
H	2.364547000	-2.662105000	-5.030761000
H	2.009384000	-1.342584000	-6.156170000
H	0.676275000	-2.190555000	-5.354313000
C	6.027004000	0.808704000	2.588056000
C	1.797928000	-0.768839000	-4.079156000
H	1.108896000	0.063241000	-4.291206000
C	3.227491000	-0.202196000	-4.009819000
H	3.303570000	0.558077000	-3.225511000
H	3.492189000	0.260700000	-4.972376000
H	3.954889000	-0.998390000	-3.799736000
C	-0.146244000	-2.563337000	-2.718841000
H	0.239387000	-3.266233000	-3.473886000
C	2.645696000	3.627097000	1.561410000
H	3.653342000	4.034217000	1.748801000
C	3.967906000	3.205340000	-1.009454000
H	4.388459000	4.055213000	-0.445831000
C	3.123577000	3.755880000	-2.175179000
H	2.679404000	2.933388000	-2.748893000
H	3.765396000	4.350139000	-2.843619000
H	2.304119000	4.398982000	-1.832078000
C	-0.541924000	-3.363881000	-1.465495000
H	0.303782000	-3.938970000	-1.067859000
H	-1.344278000	-4.072022000	-1.722681000
H	-0.911799000	-2.697165000	-0.678256000
C	-1.352520000	-1.806817000	-3.305588000
H	-1.735161000	-1.077029000	-2.582696000
H	-2.161265000	-2.515223000	-3.538425000
H	-1.100761000	-1.271880000	-4.231673000
C	5.138407000	2.352538000	-1.536722000
H	5.845751000	2.093636000	-0.740673000
H	5.679771000	2.916391000	-2.311565000
H	4.780750000	1.418586000	-1.987120000
C	2.096010000	3.056625000	2.880523000
H	1.144862000	2.539870000	2.714433000
H	1.924240000	3.877055000	3.593687000
H	2.800440000	2.348458000	3.334234000
C	1.772901000	4.776659000	1.021192000
H	2.243324000	5.280738000	0.167007000
H	1.631438000	5.527533000	1.812862000
H	0.784487000	4.413799000	0.720371000
H	4.096213000	-5.489920000	-2.214045000
H	4.018709000	-2.949090000	2.194451000
H	5.670143000	-3.107290000	1.595055000
H	6.813994000	1.205891000	3.227341000
H	1.636184000	1.223429000	-1.914315000
H	-0.172042000	-0.676616000	0.077314000
N	-1.650107000	2.163886000	2.094283000
N	-1.127083000	3.175418000	1.907515000

$TS_{EF'}$(open-shell singet)

Ti	-1.343222000	0.621475000	0.559229000
P	-1.386549000	-0.997381000	2.573532000
P	-2.870644000	2.263388000	-0.761913000
N	-3.004040000	-0.628747000	0.065331000
C	-3.845098000	-0.331943000	-1.046243000
C	-4.730529000	1.323644000	-2.655139000
H	-4.735577000	2.348606000	-3.028647000
C	-3.860807000	-4.283167000	2.156424000
C	-3.266211000	-1.867568000	0.719659000
C	-4.694144000	-1.291346000	-1.667093000
C	-4.133976000	-2.861410000	0.183307000
C	-4.438266000	-4.018773000	0.911226000
H	-5.124979000	-4.740951000	0.466033000
C	-4.650665000	-2.730124000	-1.225862000
C	-2.641988000	-2.173273000	1.967256000
C	-2.938071000	-3.361761000	2.658113000
H	-2.429304000	-3.570152000	3.598608000
C	-5.536055000	-0.929689000	-2.726888000
H	-6.172739000	-1.701218000	-3.163510000
C	-3.887821000	0.991387000	-1.580496000
C	-1.896714000	-1.217988000	5.458924000
H	-2.414524000	-2.180865000	5.352682000
H	-2.330277000	-0.709441000	6.333575000
H	-0.840187000	-1.412669000	5.680799000
C	-5.567302000	0.370515000	-3.240089000
C	-2.092426000	-0.330392000	4.214560000
H	-1.543226000	0.610358000	4.373803000
C	-3.587877000	0.003689000	4.032898000
H	-3.772071000	0.594919000	3.128583000
H	-3.948486000	0.578510000	4.898968000
H	-4.181608000	-0.916815000	3.958752000
C	0.059329000	-2.082664000	3.097554000
H	-0.310549000	-2.701560000	3.930094000
C	-2.166697000	3.369454000	-2.123022000
H	-3.002955000	4.003867000	-2.462908000
C	-4.268533000	3.337273000	-0.036757000
H	-4.944546000	3.484952000	-0.895291000
C	-3.835683000	4.721910000	0.480942000
H	-3.079321000	4.646028000	1.272866000
H	-4.711267000	5.235492000	0.906159000
H	-3.438231000	5.357872000	-0.319397000
C	0.513394000	-3.015588000	1.961128000
H	-0.292685000	-3.687991000	1.643144000
H	1.356872000	-3.630315000	2.309480000
H	0.846710000	-2.438861000	1.090811000
C	1.223728000	-1.208031000	3.602286000
H	1.625010000	-0.599491000	2.783218000
H	2.031365000	-1.850762000	3.983303000
H	0.921651000	-0.532031000	4.414722000
C	-5.035324000	2.558561000	1.048947000
H	-5.343204000	1.565215000	0.699251000
H	-5.939571000	3.117233000	1.333239000
H	-4.421704000	2.434427000	1.950464000
C	-1.614895000	2.569327000	-3.318377000
H	-0.784471000	1.929281000	-2.993854000
H	-1.229178000	3.273678000	-4.071137000
H	-2.379251000	1.943056000	-3.792873000
C	-1.046033000	4.260138000	-1.544554000
H	-1.371042000	4.861771000	-0.687270000
H	-0.686336000	4.947708000	-2.324558000
H	-0.207196000	3.630300000	-1.224749000
H	-4.101197000	-5.192285000	2.705125000
H	-3.989623000	-3.301062000	-1.905182000
H	-5.645251000	-3.192511000	-1.319187000
H	-6.224354000	0.631886000	-4.067892000
H	0.417315000	0.865193000	1.157163000
H	-0.365544000	1.317549000	-0.792635000
Ti	1.316644000	0.440868000	-0.448710000
P	1.298002000	-1.233487000	-2.392814000
P	2.977700000	2.264615000	0.377343000
N	3.011727000	-0.736601000	-0.024557000
C	4.118069000	-0.263196000	0.732136000
C	5.499537000	1.603739000	1.529551000
H	5.662821000	2.678331000	1.618866000
C	3.452558000	-4.697398000	-1.580749000
C	3.151404000	-2.067041000	-0.511355000

C	5.054706000	-1.147911000	1.337836000
C	4.019693000	-3.013934000	0.095694000
C	4.170905000	-4.295021000	-0.449374000
H	4.854081000	-4.991805000	0.039491000
C	4.727424000	-2.620181000	1.367612000
C	2.419815000	-2.484002000	-1.661280000
C	2.570825000	-3.785272000	-2.171432000
H	1.995845000	-4.086347000	-3.046870000
C	6.211768000	-0.652594000	1.949429000
H	6.918253000	-1.363504000	2.381527000
C	4.333814000	1.135182000	0.897373000
C	2.054777000	-1.648516000	-5.191195000
H	2.458493000	-2.644928000	-4.961038000
H	2.636972000	-1.247395000	-6.035045000
H	1.017626000	-1.763277000	-5.531387000
C	6.461637000	0.722338000	2.033007000
C	2.190657000	-0.699870000	-3.985767000
H	1.725277000	0.268490000	-4.224283000
C	3.678942000	-0.456595000	-3.668376000
H	3.795711000	0.136534000	-2.754502000
H	4.155932000	0.081838000	-4.501102000
H	4.205499000	-1.410338000	-3.528449000
C	-0.167829000	-2.238412000	-3.017633000
H	0.222731000	-2.917294000	-3.791548000
C	2.839989000	3.331873000	1.945654000
H	3.868117000	3.667679000	2.157064000
C	3.806747000	3.503544000	-0.808450000
H	4.325423000	4.225855000	-0.155151000
C	2.760793000	4.249023000	-1.660306000
H	2.214944000	3.530407000	-2.285555000
H	3.267389000	4.974030000	-2.316127000
H	2.030796000	4.796842000	-1.052983000
C	-0.807339000	-3.085167000	-1.903700000
H	-0.089035000	-3.785978000	-1.460994000
H	-1.639719000	-3.670744000	-2.323929000
H	-1.200243000	-2.444786000	-1.106024000
C	-1.202049000	-1.295244000	-3.663538000
H	-1.604550000	-0.600109000	-2.916984000
H	-2.040408000	-1.878419000	-4.073006000
H	-0.771832000	-0.703567000	-4.483656000
C	4.845886000	2.841609000	-1.730714000
H	5.628140000	2.317234000	-1.169453000
H	5.323263000	3.613989000	-2.353308000
H	4.357321000	2.123709000	-2.399793000
C	2.355386000	2.488753000	3.137867000
H	1.357670000	2.077240000	2.944300000
H	2.304431000	3.116134000	4.041207000
H	3.039242000	1.654386000	3.339135000
C	1.966525000	4.584665000	1.742077000
H	2.420495000	5.287663000	1.032075000
H	1.853863000	5.111476000	2.701999000
H	0.963911000	4.322615000	1.385485000
H	3.573266000	-5.699387000	-1.990067000
H	4.068854000	-2.827579000	2.233795000
H	5.633894000	-3.224154000	1.518569000
H	7.370721000	1.097383000	2.500844000
H	1.893226000	1.321149000	-1.864846000
H	-0.177929000	-0.667433000	-0.065433000
N	-1.785740000	2.077724000	2.255062000
N	-1.080195000	2.973519000	2.224645000

$TS_{EF'}$(triplet)

Ti	-1.274845000	0.602172000	0.571473000
P	-1.517163000	-1.030196000	2.596853000
P	-2.786655000	2.284480000	-0.709320000
N	-2.937857000	-0.672371000	-0.014201000
C	-3.788982000	-0.308436000	-1.083246000
C	-4.723926000	1.435333000	-2.563677000
H	-4.738016000	2.478644000	-2.882980000
C	-3.793877000	-4.413098000	1.903102000
C	-3.207946000	-1.926024000	0.588132000
C	-4.646742000	-1.235263000	-1.748334000
C	-4.046453000	-2.910947000	-0.012004000
C	-4.344044000	-4.105187000	0.653377000
H	-5.003007000	-4.821077000	0.158393000
C	-4.538817000	-2.701886000	-1.420998000
C	-2.631593000	-2.262732000	1.852460000
C	-2.921475000	-3.487779000	2.481113000
H	-2.448735000	-3.719928000	3.435119000
C	-5.528847000	-0.813700000	-2.748075000
H	-6.173011000	-1.560225000	-3.216496000
C	-3.844498000	1.046939000	-1.534943000
C	-2.450359000	-1.331433000	5.363538000
H	-2.937795000	-2.290327000	5.140771000
H	-3.020975000	-0.854757000	6.175452000
H	-1.441174000	-1.532818000	5.745005000
C	-5.583098000	0.519814000	-3.172976000
C	-2.448774000	-0.403962000	4.134357000
H	-1.925898000	0.527501000	4.401077000
C	-3.893085000	-0.048707000	3.727266000
H	-3.920598000	0.557747000	2.814099000
H	-4.383897000	0.514770000	4.534951000
H	-4.475155000	-0.960862000	3.540021000
C	-0.087767000	-2.028251000	3.312648000
H	-0.516811000	-2.674656000	4.094093000
C	-2.054249000	3.359152000	-2.093676000
H	-2.858082000	4.054418000	-2.389846000
C	-4.139758000	3.451059000	-0.033280000
H	-4.805032000	3.592549000	-0.900969000
C	-3.653558000	4.839463000	0.424221000
H	-2.925532000	4.769805000	1.242280000
H	-4.514061000	5.419126000	0.792354000
H	-3.199350000	5.410698000	-0.395019000
C	0.578928000	-2.925787000	2.255024000
H	-0.137494000	-3.627113000	1.809909000
H	1.382025000	-3.510529000	2.729887000
H	1.015462000	-2.324242000	1.449105000
C	0.936934000	-1.076687000	3.962848000
H	1.378181000	-0.415347000	3.206512000
H	1.748392000	-1.658611000	4.425075000
H	0.487650000	-0.448642000	4.745386000
C	-4.948156000	2.754799000	1.076126000
H	-5.289701000	1.759245000	0.764998000
H	-5.833981000	3.358701000	1.324823000
H	-4.350896000	2.645862000	1.990319000
C	-1.606973000	2.553971000	-3.327602000
H	-0.806393000	1.856277000	-3.052160000
H	-1.209955000	3.248891000	-4.083943000
H	-2.429363000	1.986849000	-3.778796000
C	-0.856194000	4.164941000	-1.548995000
H	-1.100042000	4.742031000	-0.648249000
H	-0.503426000	4.868532000	-2.318727000
H	-0.034807000	3.478053000	-1.306428000
H	-4.022098000	-5.354955000	2.399544000
H	-3.830711000	-3.179459000	-2.125611000
H	-5.503641000	-3.208033000	-1.576711000
H	-6.269559000	0.830997000	-3.958822000
H	0.485745000	1.059879000	1.083157000
H	-0.349230000	1.051427000	-0.969635000
Ti	1.332780000	0.424516000	-0.405893000
P	1.291986000	-1.172690000	-2.412267000
P	3.061336000	2.219211000	0.406267000
N	3.015318000	-0.763216000	-0.011531000
C	4.053989000	-0.344943000	0.863764000
C	5.342453000	1.459533000	1.926714000
H	5.494975000	2.524881000	2.101292000
C	3.589809000	-4.584503000	-1.826466000
C	3.181424000	-2.056542000	-0.574767000

C	4.926612000	-1.273718000	1.497180000
C	4.030965000	-3.034432000	0.007872000
C	4.242117000	-4.262061000	-0.630889000
H	4.912823000	-4.984709000	-0.163197000
C	4.632261000	-2.746874000	1.360922000
C	2.493310000	-2.400691000	-1.773622000
C	2.699836000	-3.655205000	-2.375257000
H	2.154927000	-3.909221000	-3.283589000
C	6.000375000	-0.825359000	2.274174000
H	6.658882000	-1.567649000	2.728253000
C	4.267795000	1.040259000	1.121950000
C	1.946706000	-1.489746000	-5.248269000
H	2.494491000	-2.423560000	-5.059566000
H	2.412147000	-1.009207000	-6.122343000
H	0.913852000	-1.739851000	-5.521273000
C	6.227915000	0.538645000	2.493952000
C	2.035486000	-0.536786000	-4.041319000
H	1.445248000	0.369353000	-4.249174000
C	3.496251000	-0.114447000	-3.801581000
H	3.566901000	0.548254000	-2.931919000
H	3.882801000	0.419847000	-4.682405000
H	4.132592000	-0.992211000	-3.623964000
C	-0.157430000	-2.231538000	-2.978119000
H	0.234401000	-2.887475000	-3.771404000
C	2.790327000	3.420694000	1.845814000
H	3.788916000	3.828158000	2.076111000
C	4.071613000	3.324235000	-0.777800000
H	4.439396000	4.145081000	-0.139351000
C	3.187894000	3.922343000	-1.890157000
H	2.784470000	3.126577000	-2.528270000
H	3.789600000	4.605880000	-2.508534000
H	2.337056000	4.487183000	-1.489864000
C	-0.698719000	-3.113394000	-1.840365000
H	0.075032000	-3.781359000	-1.442116000
H	-1.521573000	-3.736245000	-2.222552000
H	-1.080378000	-2.497709000	-1.018960000
C	-1.257996000	-1.334435000	-3.575892000
H	-1.645905000	-0.643557000	-2.818544000
H	-2.094239000	-1.953917000	-3.931989000
H	-0.895027000	-0.741369000	-4.426953000
C	5.292189000	2.602505000	-1.379971000
H	5.996435000	2.270457000	-0.608841000
H	5.819443000	3.290483000	-2.058156000
H	4.989632000	1.724082000	-1.962342000
C	2.256357000	2.700248000	3.095957000
H	1.295558000	2.216340000	2.886162000
H	2.106476000	3.430363000	3.905625000
H	2.958693000	1.935188000	3.449495000
C	1.879882000	4.594082000	1.435222000
H	2.319747000	5.194459000	0.628243000
H	1.727080000	5.258734000	2.298506000
H	0.896834000	4.235448000	1.108901000
H	3.756102000	-5.546219000	-2.309377000
H	3.915235000	-3.048958000	2.148241000
H	5.539896000	-3.345571000	1.524720000
H	7.066008000	0.873716000	3.102939000
H	1.735346000	1.332618000	-1.825224000
H	0.004943000	-0.764881000	0.089812000
N	-1.694364000	2.071416000	2.380959000
N	-1.213618000	3.096477000	2.281234000

F'(closed-shell singlet)

Ti	-1.306073000	0.774164000	0.689542000
P	-1.346699000	-0.821803000	2.683738000
P	-2.798381000	2.124077000	-0.945129000
N	-2.965047000	-0.633072000	0.160192000
C	-3.856471000	-0.423385000	-0.929931000
C	-4.860528000	1.118835000	-2.588948000
H	-4.887246000	2.115778000	-3.032221000
C	-3.540058000	-4.304187000	2.347267000
C	-3.142309000	-1.868240000	0.849365000
C	-4.711574000	-1.432610000	-1.466766000
C	-3.967310000	-2.929220000	0.367277000
C	-4.172324000	-4.092487000	1.119352000
H	-4.827602000	-4.861025000	0.704707000
C	-4.558935000	-2.857980000	-1.014097000
C	-2.483083000	-2.113169000	2.094376000
C	-2.677790000	-3.308317000	2.810067000
H	-2.138711000	-3.459102000	3.744578000
C	-5.634301000	-1.139405000	-2.478334000
H	-6.274303000	-1.948110000	-2.836634000
C	-3.940071000	0.853331000	-1.561166000
C	-2.144333000	-1.024181000	5.501597000
H	-2.688087000	-1.964931000	5.339637000
H	-2.641650000	-0.498097000	6.331208000
H	-1.124437000	-1.262764000	5.830349000
C	-5.735106000	0.132975000	-3.050483000
C	-2.174868000	-0.131441000	4.247370000
H	-1.614110000	0.792530000	4.449523000
C	-3.626050000	0.261242000	3.906816000
H	-3.674783000	0.890484000	3.010081000
H	-4.067860000	0.824309000	4.742519000
H	-4.240647000	-0.631775000	3.728708000
C	0.134371000	-1.772662000	3.359542000
H	-0.251962000	-2.419252000	4.162825000
C	-2.118552000	2.981547000	-2.486225000
H	-2.959913000	3.561771000	-2.902193000
C	-4.076169000	3.377861000	-0.291969000
H	-4.807653000	3.443899000	-1.114357000
C	-3.546940000	4.794490000	0.000649000
H	-2.720586000	4.773377000	0.721685000
H	-4.361362000	5.397817000	0.430838000
H	-3.208282000	5.304176000	-0.910087000
C	0.771223000	-2.667531000	2.283890000
H	0.052973000	-3.393060000	1.883270000
H	1.616678000	-3.223160000	2.718778000
H	1.152161000	-2.062414000	1.451591000
C	1.168724000	-0.803510000	3.965862000
H	1.581051000	-0.146509000	3.190333000
H	1.998734000	-1.373931000	4.409747000
H	0.736539000	-0.171287000	4.753687000
C	-4.796974000	2.797561000	0.940642000
H	-5.159154000	1.777218000	0.759915000
H	-5.663368000	3.428090000	1.191323000
H	-4.131006000	2.784390000	1.812482000
C	-1.638629000	1.961091000	-3.535372000
H	-0.819870000	1.357896000	-3.119828000
H	-1.253021000	2.498962000	-4.415292000
H	-2.441932000	1.291094000	-3.863236000
C	-0.959734000	3.937921000	-2.137494000
H	-1.225533000	4.677869000	-1.375051000
H	-0.650136000	4.477718000	-3.045791000
H	-0.106152000	3.358017000	-1.769016000
H	-3.700330000	-5.219925000	2.914199000
H	-3.896919000	-3.395527000	-1.721760000
H	-5.524130000	-3.386187000	-1.052301000
H	-6.456498000	0.341109000	-3.839040000
H	0.537157000	0.747970000	1.181803000
H	-0.162540000	1.515134000	-0.557043000
Ti	1.264062000	0.331520000	-0.434735000
P	1.262504000	-1.373293000	-2.370261000
P	2.806627000	2.295178000	0.291535000
N	3.027119000	-0.682208000	-0.030393000
C	4.015634000	-0.159563000	0.853451000
C	5.089285000	1.773086000	1.917996000
H	5.133913000	2.849162000	2.083311000
C	3.915856000	-4.499626000	-1.741983000
C	3.299116000	-1.975272000	-0.563068000

C	4.964117000	-0.991419000	1.504852000
C	4.241298000	-2.854306000	0.034678000
C	4.555319000	-4.076912000	-0.572078000
H	5.299190000	-4.717450000	-0.095762000
C	4.833514000	-2.487928000	1.372688000
C	2.620435000	-2.427135000	-1.733326000
C	2.928906000	-3.678474000	-2.296457000
H	2.386751000	-4.016139000	-3.178447000
C	5.968895000	-0.431094000	2.303122000
H	6.690444000	-1.098642000	2.776632000
C	4.081729000	1.241590000	1.094179000
C	1.748699000	-1.836862000	-5.208558000
H	2.447077000	-2.661700000	-5.012130000
H	2.053899000	-1.369332000	-6.156731000
H	0.745261000	-2.254987000	-5.355328000
C	6.047923000	0.949170000	2.515972000
C	1.803800000	-0.779437000	-4.088987000
H	1.085494000	0.023404000	-4.316144000
C	3.209788000	-0.157892000	-4.009130000
H	3.246720000	0.617167000	-3.236371000
H	3.469083000	0.299434000	-4.975542000
H	3.964144000	-0.922250000	-3.777277000
C	-0.120157000	-2.601917000	-2.720770000
H	0.277517000	-3.308433000	-3.466127000
C	2.490253000	3.613372000	1.612582000
H	3.474136000	4.085451000	1.774445000
C	3.808959000	3.302726000	-0.984124000
H	4.201012000	4.158709000	-0.409502000
C	2.930451000	3.839511000	-2.130212000
H	2.504498000	3.010462000	-2.708549000
H	3.544924000	4.459611000	-2.800634000
H	2.098336000	4.454706000	-1.768952000
C	-0.509325000	-3.389328000	-1.456988000
H	0.340719000	-3.952365000	-1.051609000
H	-1.305347000	-4.106806000	-1.706227000
H	-0.886515000	-2.716000000	-0.678857000
C	-1.335177000	-1.870612000	-3.322875000
H	-1.749380000	-1.154309000	-2.604104000
H	-2.121693000	-2.599367000	-3.567510000
H	-1.084655000	-1.328481000	-4.245022000
C	5.005676000	2.508819000	-1.544215000
H	5.735722000	2.263219000	-0.764831000
H	5.510886000	3.109949000	-2.315269000
H	4.678973000	1.570410000	-2.008881000
C	2.018404000	3.001731000	2.943858000
H	1.068061000	2.472856000	2.822016000
H	1.868861000	3.807310000	3.678507000
H	2.758021000	2.301485000	3.351238000
C	1.520602000	4.705191000	1.116957000
H	1.908043000	5.230204000	0.234294000
H	1.387313000	5.452748000	1.913320000
H	0.536039000	4.285909000	0.880475000
H	4.163596000	-5.456620000	-2.198189000
H	4.173699000	-2.868315000	2.175655000
H	5.806310000	-2.979704000	1.517839000
H	6.832778000	1.372777000	3.140542000
H	1.594075000	1.219114000	-1.873363000
H	-0.248903000	-0.599357000	-0.092899000
N	-1.441125000	2.110845000	2.328081000
N	-1.277842000	2.781650000	1.355967000

F'(triplet)

Ti	-1.305090000	0.740998000	0.494827000
P	-1.488010000	-0.509515000	2.763074000
P	-2.915179000	2.003428000	-1.144543000
N	-2.908457000	-0.731766000	0.131438000
C	-3.812137000	-0.627962000	-0.949580000
C	-4.938306000	0.759224000	-2.658309000
H	-5.036913000	1.724050000	-3.158483000
C	-3.237194000	-4.245146000	2.574871000
C	-3.014373000	-1.906983000	0.910726000
C	-4.605277000	-1.720736000	-1.415717000
C	-3.745495000	-3.059925000	0.494599000
C	-3.862752000	-4.179662000	1.324588000
H	-4.441518000	-5.031081000	0.961387000
C	-4.331276000	-3.106411000	-0.892502000
C	-2.386277000	-1.985580000	2.193353000
C	-2.491249000	-3.140434000	2.990916000
H	-1.980770000	-3.170820000	3.952974000
C	-5.566339000	-1.538864000	-2.414880000
H	-6.160358000	-2.402052000	-2.721279000
C	-3.981744000	0.612547000	-1.636777000
C	-2.587952000	-0.535695000	5.471350000
H	-2.933074000	-1.572140000	5.354182000
H	-3.278645000	-0.036975000	6.168410000
H	-1.596784000	-0.547722000	5.942567000
C	-5.758084000	-0.302338000	-3.044645000
C	-2.601960000	0.213837000	4.125795000
H	-2.214132000	1.231529000	4.282373000
C	-4.044203000	0.321779000	3.590874000
H	-4.078368000	0.800513000	2.605800000
H	-4.655222000	0.914947000	4.287524000
H	-4.496164000	-0.674902000	3.499590000
C	0.003381000	-1.165509000	3.704872000
H	-0.392631000	-1.766408000	4.538081000
C	-2.245733000	2.708269000	-2.773433000
H	-3.086556000	3.254970000	-3.233614000
C	-4.239954000	3.291381000	-0.674340000
H	-4.905224000	3.312657000	-1.553471000
C	-3.711941000	4.720202000	-0.441745000
H	-2.946478000	4.752102000	0.344259000
H	-4.544717000	5.364952000	-0.121851000
H	-3.289795000	5.158143000	-1.354424000
C	0.878316000	-2.071035000	2.822087000
H	0.312936000	-2.922243000	2.423680000
H	1.717484000	-2.461757000	3.418371000
H	1.293998000	-1.506703000	1.977746000
C	0.823890000	0.003707000	4.285192000
H	1.236672000	0.617747000	3.475336000
H	1.662921000	-0.388513000	4.878955000
H	0.224513000	0.652587000	4.939226000
C	-5.063557000	2.802703000	0.532575000
H	-5.445311000	1.785960000	0.376333000
H	-5.923552000	3.472311000	0.685366000
H	-4.464753000	2.811433000	1.451777000
C	-1.778932000	1.598387000	-3.735079000
H	-0.962561000	1.024412000	-3.277039000
H	-1.396993000	2.058985000	-4.659355000
H	-2.589167000	0.909443000	-4.000573000
C	-1.077920000	3.684655000	-2.519530000
H	-1.334629000	4.493958000	-1.825863000
H	-0.769905000	4.141284000	-3.472703000
H	-0.223361000	3.135175000	-2.106736000
H	-3.322922000	-5.132328000	3.200212000
H	-3.618304000	-3.614487000	-1.570718000
H	-5.246067000	-3.718380000	-0.908501000
H	-6.506378000	-0.179978000	-3.826048000
H	0.460715000	0.955873000	1.095897000
H	-0.277038000	1.199390000	-0.957891000
Ti	1.287314000	0.283380000	-0.453428000
P	1.431224000	-1.612943000	-2.178202000
P	2.786391000	2.368802000	0.038901000
N	3.071419000	-0.626076000	0.123137000
C	4.001335000	0.026669000	0.976842000
C	4.980040000	2.103421000	1.844193000
H	4.997098000	3.192440000	1.877046000
C	4.241555000	-4.514174000	-1.208969000
C	3.432124000	-1.941971000	-0.280027000

C	4.947952000	-0.692707000	1.755393000
C	4.386614000	-2.713760000	0.436032000
C	4.796556000	-3.961502000	-0.048960000
H	5.547289000	-4.518173000	0.514431000
C	4.876727000	-2.199638000	1.767702000
C	2.829417000	-2.531243000	-1.429814000
C	3.236694000	-3.802419000	-1.872716000
H	2.754258000	-4.244421000	-2.743639000
C	5.898264000	-0.012730000	2.525737000
H	6.618442000	-0.596896000	3.100918000
C	4.026159000	1.449810000	1.043325000
C	1.871678000	-2.341930000	-4.975950000
H	2.568917000	-3.150711000	-4.717588000
H	2.165765000	-1.962731000	-5.966355000
H	0.864961000	-2.766670000	-5.071414000
C	5.927078000	1.385267000	2.580851000
C	1.946679000	-1.188161000	-3.956617000
H	1.226511000	-0.406986000	-4.245073000
C	3.355157000	-0.567185000	-3.960939000
H	3.411006000	0.269587000	-3.257134000
H	3.593894000	-0.193510000	-4.967976000
H	4.112972000	-1.311897000	-3.681463000
C	0.112023000	-2.939959000	-2.398130000
H	0.530044000	-3.690201000	-3.087480000
C	2.431048000	3.873764000	1.135882000
H	3.406864000	4.372834000	1.259221000
C	3.838168000	3.190393000	-1.327445000
H	4.202029000	4.128846000	-0.876208000
C	2.998457000	3.534307000	-2.573203000
H	2.598106000	2.620572000	-3.029363000
H	3.631270000	4.051876000	-3.310363000
H	2.148624000	4.187272000	-2.339865000
C	-0.220660000	-3.632872000	-1.064561000
H	0.658405000	-4.133264000	-0.639130000
H	-0.999342000	-4.392587000	-1.229874000
H	-0.600735000	-2.910402000	-0.332513000
C	-1.143615000	-2.312812000	-3.033631000
H	-1.579146000	-1.564858000	-2.360185000
H	-1.898336000	-3.091806000	-3.217009000
H	-0.929945000	-1.824948000	-3.994739000
C	5.060867000	2.334570000	-1.712501000
H	5.762590000	2.226936000	-0.877596000
H	5.590433000	2.811074000	-2.551452000
H	4.758662000	1.329235000	-2.030701000
C	1.910943000	3.473000000	2.527094000
H	0.975948000	2.909500000	2.446076000
H	1.717221000	4.379287000	3.120948000
H	2.640130000	2.858138000	3.068625000
C	1.482052000	4.872229000	0.442820000
H	1.913668000	5.274529000	-0.482577000
H	1.294876000	5.721813000	1.116778000
H	0.519344000	4.405825000	0.209324000
H	4.563708000	-5.489505000	-1.570330000
H	4.176960000	-2.527740000	2.560050000
H	5.853828000	-2.635336000	2.022101000
H	6.670183000	1.903944000	3.184644000
H	1.731069000	0.957545000	-1.981416000
H	-0.211692000	-0.690453000	0.000575000
N	-2.038403000	2.411256000	2.033395000
N	-1.221645000	2.867782000	1.358310000

$TS_{F'G'}$(closed-shell singlet)

Ti	1.222237000	0.506314000	-0.561088000
P	1.587857000	-1.408367000	-2.313608000
P	2.629726000	2.480831000	0.364014000
N	3.070798000	-0.491863000	0.068047000
C	3.949488000	0.118692000	1.009797000
C	4.854808000	2.149704000	2.080311000
H	4.822218000	3.232925000	2.202131000
C	4.293251000	-4.369815000	-1.303593000
C	3.457150000	-1.796871000	-0.340107000
C	4.896936000	-0.623627000	1.774987000
C	4.392865000	-2.595586000	0.378133000
C	4.813073000	-3.834449000	-0.119706000
H	5.544837000	-4.401643000	0.458373000
C	4.849759000	-2.127936000	1.733653000
C	2.904364000	-2.373555000	-1.522946000
C	3.315023000	-3.637858000	-1.982043000
H	2.858524000	-4.053158000	-2.879958000
C	5.818241000	0.021570000	2.607661000
H	6.535263000	-0.591683000	3.156357000
C	3.930210000	1.529123000	1.221346000
C	2.686704000	-1.837549000	-4.977485000
H	3.473096000	-2.500130000	-4.591287000
H	3.077964000	-1.350058000	-5.883431000
H	1.828423000	-2.452083000	-5.279226000
C	5.821816000	1.411470000	2.766429000
C	2.309807000	-0.762200000	-3.942547000
H	1.507626000	-0.130513000	-4.354536000
C	3.515812000	0.143898000	-3.627465000
H	3.226394000	0.971753000	-2.968067000
H	3.914580000	0.575700000	-4.557561000
H	4.319830000	-0.423648000	-3.139153000
C	0.305704000	-2.673900000	-2.861746000
H	0.827966000	-3.349566000	-3.557624000
C	2.011213000	3.625987000	1.737016000
H	2.910825000	4.156458000	2.091017000
C	3.598016000	3.713481000	-0.729302000
H	3.843123000	4.548243000	-0.050517000
C	2.744650000	4.256280000	-1.894151000
H	2.538014000	3.469538000	-2.627985000
H	3.290995000	5.068336000	-2.398083000
H	1.777887000	4.653482000	-1.562783000
C	-0.217067000	-3.510067000	-1.679853000
H	0.594703000	-4.047241000	-1.174231000
H	-0.940653000	-4.251864000	-2.050543000
H	-0.722154000	-2.874290000	-0.944009000
C	-0.851143000	-1.989900000	-3.618791000
H	-1.393661000	-1.300812000	-2.961062000
H	-1.555315000	-2.756470000	-3.976050000
H	-0.502946000	-1.423379000	-4.493000000
C	4.919856000	3.127456000	-1.263723000
H	5.603123000	2.846056000	-0.454816000
H	5.418958000	3.878581000	-1.894759000
H	4.742424000	2.237733000	-1.881358000
C	1.411450000	2.828567000	2.908271000
H	0.516849000	2.280634000	2.585257000
H	1.126238000	3.526453000	3.711111000
H	2.135214000	2.113983000	3.319995000
C	1.010003000	4.670830000	1.212740000
H	1.458734000	5.347849000	0.474492000
H	0.653011000	5.285649000	2.052743000
H	0.144281000	4.175204000	0.758498000
H	4.622950000	-5.339864000	-1.671999000
H	4.140485000	-2.492511000	2.502222000
H	5.827797000	-2.559915000	1.991997000
H	6.544358000	1.900712000	3.417678000
H	-0.024083000	-0.818463000	-0.215655000
H	-0.134937000	1.769448000	0.016970000
Ti	-1.252040000	0.405710000	0.414164000
P	-1.289857000	-1.171777000	2.396540000
P	-3.043195000	2.199733000	-0.408095000
N	-2.972952000	-0.770563000	0.012923000
C	-4.059130000	-0.352784000	-0.804463000
C	-5.457322000	1.449443000	-1.721063000
H	-5.637910000	2.516166000	-1.858684000
C	-3.408941000	-4.681502000	1.697868000
C	-3.104013000	-2.088934000	0.540586000

C	-4.937822000	-1.282368000	-1.429691000
C	-3.929656000	-3.072421000	-0.066041000
C	-4.086067000	-4.333196000	0.524006000
H	-4.736560000	-5.059580000	0.033966000
C	-4.574024000	-2.745138000	-1.389103000
C	-2.405215000	-2.455277000	1.727874000
C	-2.557364000	-3.737638000	2.282794000
H	-2.002210000	-4.000718000	3.182696000
C	-6.073636000	-0.839152000	-2.115831000
H	-6.734438000	-1.583196000	-2.563640000
C	-4.320012000	1.032858000	-1.005647000
C	-2.217112000	-1.498871000	5.135821000
H	-2.756273000	-2.417751000	4.866038000
H	-2.763869000	-1.028093000	5.966984000
H	-1.222680000	-1.774022000	5.509883000
C	-6.357659000	0.524727000	-2.257975000
C	-2.158079000	-0.520947000	3.948122000
H	-1.560036000	0.360794000	4.225275000
C	-3.570123000	-0.043922000	3.566396000
H	-3.523779000	0.643121000	2.713876000
H	-4.034631000	0.479297000	4.415522000
H	-4.211194000	-0.892858000	3.291922000
C	0.182771000	-2.118838000	3.082666000
H	-0.224514000	-2.806579000	3.840604000
C	-2.888953000	3.399252000	-1.881179000
H	-3.844769000	3.950649000	-1.878397000
C	-3.920586000	3.381815000	0.823492000
H	-4.188720000	4.254020000	0.205241000
C	-2.976020000	3.862631000	1.941602000
H	-2.667721000	3.027557000	2.581117000
H	-3.494160000	4.614136000	2.557427000
H	-2.062453000	4.319120000	1.542764000
C	0.878647000	-2.947425000	1.990480000
H	0.195050000	-3.675805000	1.537549000
H	1.724156000	-3.498631000	2.429264000
H	1.263211000	-2.293982000	1.199589000
C	1.170591000	-1.156339000	3.771864000
H	1.590667000	-0.452161000	3.044009000
H	1.997983000	-1.732206000	4.212834000
H	0.698319000	-0.578228000	4.578073000
C	-5.223223000	2.809335000	1.414989000
H	-5.960343000	2.567582000	0.641281000
H	-5.666133000	3.555924000	2.091752000
H	-5.038257000	1.899061000	1.996968000
C	-2.738992000	2.717469000	-3.253385000
H	-1.840335000	2.093329000	-3.297757000
H	-2.659806000	3.495747000	-4.028105000
H	-3.606152000	2.089278000	-3.488829000
C	-1.752696000	4.409243000	-1.629061000
H	-1.893469000	4.966474000	-0.693030000
H	-1.720650000	5.140433000	-2.450715000
H	-0.783257000	3.898821000	-1.587009000
H	-3.531270000	-5.669433000	2.139218000
H	-3.861093000	-2.965303000	-2.207047000
H	-5.455582000	-3.377353000	-1.567755000
H	-7.244281000	0.857034000	-2.795589000
H	-1.385585000	1.399450000	1.821385000
H	0.458199000	0.440965000	1.149331000
N	-0.201913000	0.984322000	-2.182452000
N	0.771949000	1.662400000	-2.277324000

$TS_{F'G'}$(triplet)

Ti	-1.150346000	-0.531283000	0.406292000
P	-1.601042000	-2.571541000	-1.125938000
P	-2.919128000	0.464201000	2.182158000
N	-2.805279000	0.159019000	-0.767050000
C	-3.594662000	1.266156000	-0.377203000
C	-4.535312000	2.675379000	1.408535000
H	-4.627950000	2.902909000	2.471161000
C	-4.190523000	-1.829019000	-4.280320000
C	-3.213844000	-0.472799000	-1.961522000
C	-4.340845000	2.035757000	-1.313016000
C	-4.008858000	0.201403000	-2.934230000
C	-4.507562000	-0.483888000	-4.045463000
H	-5.129288000	0.061194000	-4.757907000
C	-4.216355000	1.688966000	-2.776205000
C	-2.854034000	-1.829494000	-2.230845000
C	-3.335183000	-2.477249000	-3.385727000
H	-3.028138000	-3.501707000	-3.590083000
C	-5.152636000	3.089722000	-0.879603000
H	-5.712949000	3.655981000	-1.625642000
C	-3.716460000	1.606656000	1.001844000
C	-2.583297000	-5.317352000	-1.456476000
H	-3.460379000	-5.041827000	-2.056482000
H	-2.828458000	-6.247717000	-0.921841000
H	-1.749977000	-5.537110000	-2.136402000
C	-5.251868000	3.431621000	0.476008000
C	-2.244465000	-4.215914000	-0.434181000
H	-1.399285000	-4.560581000	0.183610000
C	-3.437397000	-3.956045000	0.501747000
H	-3.178335000	-3.222538000	1.275043000
H	-3.740682000	-4.889938000	0.998397000
H	-4.300068000	-3.576159000	-0.063082000
C	-0.284795000	-3.115916000	-2.369682000
H	-0.804339000	-3.777036000	-3.081688000
C	-2.371057000	1.550828000	3.647835000
H	-3.304838000	1.804349000	4.178153000
C	-4.465788000	-0.383093000	2.917201000
H	-4.990025000	0.414753000	3.470336000
C	-4.120483000	-1.521682000	3.897750000
H	-3.484189000	-2.279768000	3.422380000
H	-5.046414000	-2.016415000	4.228069000
H	-3.604246000	-1.158289000	4.794162000
C	0.261404000	-1.902038000	-3.144242000
H	-0.538597000	-1.360921000	-3.664806000
H	0.985751000	-2.249423000	-3.897214000
H	0.766644000	-1.204390000	-2.464731000
C	0.858118000	-3.899370000	-1.700577000
H	1.388672000	-3.260302000	-0.984959000
H	1.579965000	-4.223794000	-2.464967000
H	0.504616000	-4.796861000	-1.174069000
C	-5.401907000	-0.884280000	1.800037000
H	-5.762721000	-0.058965000	1.175984000
H	-6.273401000	-1.382920000	2.250874000
H	-4.897640000	-1.607481000	1.148338000
C	-1.673963000	2.854814000	3.214500000
H	-0.757218000	2.627883000	2.655850000
H	-1.395603000	3.425587000	4.114226000
H	-2.315755000	3.488188000	2.592652000
C	-1.439075000	0.799836000	4.626072000
H	-1.818871000	-0.183218000	4.927638000
H	-1.312189000	1.405731000	5.535857000
H	-0.450301000	0.659829000	4.172964000
H	-4.574964000	-2.347186000	-5.157479000
H	-3.350331000	2.220515000	-3.212210000
H	-5.100965000	2.025318000	-3.336195000
H	-5.882701000	4.259325000	0.796616000
H	0.574740000	-1.285740000	0.112989000
H	-0.391806000	1.089774000	0.995137000
Ti	1.280112000	0.370181000	0.586404000
P	1.421950000	2.760044000	-0.356538000
P	3.075715000	-1.126573000	1.851353000
N	2.872509000	0.216640000	-0.823260000
C	3.765617000	-0.888862000	-0.828919000
C	4.971416000	-2.660297000	0.382520000
H	5.167327000	-3.193973000	1.312344000
C	3.699778000	3.163091000	-3.802975000
C	3.094343000	1.162496000	-1.856822000

C	4.471433000	-1.287775000	-1.999820000
C	3.817490000	0.845847000	-3.040377000
C	4.134575000	1.842602000	-3.969475000
H	4.709062000	1.564889000	-4.854801000
C	4.149953000	-0.600366000	-3.301864000
C	2.595579000	2.490127000	-1.729286000
C	2.900837000	3.465437000	-2.695758000
H	2.498144000	4.471538000	-2.587197000
C	5.417472000	-2.317578000	-1.951355000
H	5.944184000	-2.581646000	-2.869903000
C	4.024852000	-1.620269000	0.367873000
C	2.189123000	5.528717000	0.213440000
H	2.826154000	5.605226000	-0.678177000
H	2.612299000	6.201525000	0.974886000
H	1.189555000	5.903983000	-0.038390000
C	5.682618000	-3.014404000	-0.767327000
C	2.173627000	4.090784000	0.767517000
H	1.529840000	4.054134000	1.660174000
C	3.592556000	3.665288000	1.183004000
H	3.579296000	2.657222000	1.610417000
H	3.988265000	4.359877000	1.939222000
H	4.272457000	3.672592000	0.319657000
C	0.014628000	3.668475000	-1.224575000
H	0.477005000	4.573348000	-1.650154000
C	2.841392000	-2.785582000	2.751091000
H	3.869684000	-3.162977000	2.878092000
C	4.369837000	-0.327741000	3.006425000
H	4.814830000	-1.177059000	3.552183000
C	3.718573000	0.626888000	4.026982000
H	3.246491000	1.474733000	3.517582000
H	4.488193000	1.006313000	4.716540000
H	2.940443000	0.134584000	4.623729000
C	-0.569245000	2.838586000	-2.380855000
H	0.199385000	2.571267000	-3.116579000
H	-1.341522000	3.432918000	-2.893074000
H	-1.026763000	1.915551000	-2.005795000
C	-1.080143000	4.092159000	-0.230127000
H	-1.555361000	3.212202000	0.216251000
H	-1.858143000	4.665403000	-0.755344000
H	-0.688652000	4.720586000	0.581654000
C	5.495649000	0.376222000	2.223459000
H	6.072388000	-0.332468000	1.618110000
H	6.180981000	0.864960000	2.932524000
H	5.098701000	1.146989000	1.552082000
C	2.063933000	-3.813685000	1.910521000
H	1.045073000	-3.473856000	1.693721000
H	1.995774000	-4.760938000	2.467256000
H	2.570176000	-4.012871000	0.959031000
C	2.246303000	-2.635884000	4.166780000
H	2.885327000	-2.026545000	4.817749000
H	2.164311000	-3.632694000	4.625431000
H	1.245692000	-2.191088000	4.150000000
H	3.947754000	3.928726000	-4.536451000
H	3.278650000	-1.092408000	-3.774183000
H	4.983335000	-0.694331000	-4.012870000
H	6.419410000	-3.815759000	-0.742410000
H	1.680660000	1.373996000	1.963024000
H	0.031121000	0.301463000	-0.804925000
N	-0.719627000	-1.789049000	2.297512000
N	0.030301000	-0.899158000	2.305542000

F''(closed-shell singlet)

Ti	1.201347000	0.481619000	-0.397087000
P	1.244492000	-0.986831000	-2.454938000
P	2.949722000	2.305235000	0.437444000
N	2.930884000	-0.679176000	0.015063000
C	3.961271000	-0.252108000	0.878388000
C	5.196331000	1.560361000	2.008543000
H	5.312018000	2.624328000	2.220614000
C	3.582618000	-4.394575000	-1.963047000
C	3.133395000	-1.930211000	-0.609231000
C	4.875424000	-1.171260000	1.474144000
C	4.018174000	-2.907121000	-0.079249000
C	4.247959000	-4.105221000	-0.764807000
H	4.938436000	-4.832476000	-0.333965000
C	4.628033000	-2.648358000	1.278134000
C	2.451065000	-2.227413000	-1.827960000
C	2.674759000	-3.460243000	-2.472552000
H	2.135036000	-3.690737000	-3.390221000
C	5.929550000	-0.714515000	2.269227000
H	6.615055000	-1.448800000	2.696253000
C	4.142469000	1.136043000	1.175396000
C	2.157802000	-1.217941000	-5.248526000
H	2.762174000	-2.103369000	-5.008210000
H	2.655297000	-0.694316000	-6.079747000
H	1.177235000	-1.552376000	-5.610847000
C	6.105812000	0.649318000	2.549596000
C	2.051524000	-0.275927000	-4.035663000
H	1.399025000	0.571754000	-4.305151000
C	3.439003000	0.280424000	-3.665467000
H	3.382824000	0.925239000	-2.777712000
H	3.856192000	0.866189000	-4.498575000
H	4.134842000	-0.537706000	-3.434466000
C	-0.146981000	-2.055991000	-3.160365000
H	0.301020000	-2.660633000	-3.964060000
C	2.488998000	3.426151000	1.891463000
H	3.430965000	3.866531000	2.258931000
C	3.939652000	3.510886000	-0.659698000
H	4.184931000	4.366378000	-0.009124000
C	3.054226000	4.013927000	-1.820393000
H	2.804445000	3.190641000	-2.503748000
H	3.591328000	4.780684000	-2.398870000
H	2.112059000	4.452593000	-1.467563000
C	-0.731182000	-3.006249000	-2.101237000
H	0.034009000	-3.677438000	-1.692593000
H	-1.518902000	-3.623769000	-2.560533000
H	-1.167459000	-2.439432000	-1.271204000
C	-1.244510000	-1.164285000	-3.770829000
H	-1.709527000	-0.548488000	-2.990219000
H	-2.028973000	-1.789690000	-4.223298000
H	-0.856624000	-0.495655000	-4.552865000
C	5.256486000	2.912742000	-1.188921000
H	5.935664000	2.635927000	-0.374822000
H	5.761727000	3.654081000	-1.826559000
H	5.076503000	2.014951000	-1.793602000
C	1.850513000	2.601740000	3.023854000
H	0.944113000	2.090672000	2.665626000
H	1.568873000	3.264766000	3.856510000
H	2.541596000	1.842057000	3.408172000
C	1.552234000	4.566083000	1.449964000
H	2.013155000	5.221444000	0.698867000
H	1.294345000	5.189762000	2.319253000
H	0.622326000	4.157137000	1.033663000
H	3.759542000	-5.334784000	-2.483639000
H	3.930466000	-3.003301000	2.060903000
H	5.556823000	-3.222570000	1.409802000
H	6.926125000	0.987067000	3.181012000
H	-0.000330000	1.847778000	-0.002826000
Ti	-1.201267000	0.482122000	0.395772000
P	-1.244309000	-0.983266000	2.455942000
P	-2.950542000	2.304395000	-0.439836000
N	-2.930403000	-0.679641000	-0.014568000
C	-3.960911000	-0.253892000	-0.878412000
C	-5.196316000	1.556885000	-2.010881000
H	-5.312340000	2.620569000	-2.224171000
C	-3.581676000	-4.392270000	1.968808000
C	-3.132815000	-1.929816000	0.611511000
C	-4.874772000	-1.174019000	-1.473071000

C	-4.017397000	-2.907588000	0.082847000
C	-4.246978000	-4.104771000	0.770101000
H	-4.937286000	-4.832779000	0.340260000
C	-4.627344000	-2.650837000	-1.274888000
C	-2.450570000	-2.225078000	1.830726000
C	-2.674072000	-3.457011000	2.477083000
H	-2.134398000	-3.686068000	3.395141000
C	-5.928833000	-0.718525000	-2.268973000
H	-6.614108000	-1.453502000	-2.695175000
C	-4.142526000	1.133878000	-1.176979000
C	-2.156498000	-1.210885000	5.250298000
H	-2.760298000	-2.097154000	5.011647000
H	-2.654085000	-0.686302000	6.080860000
H	-1.175544000	-1.544001000	5.612787000
C	-6.105360000	0.644907000	-2.551099000
C	-2.051386000	-0.270700000	4.035904000
H	-1.399473000	0.577914000	4.303875000
C	-3.439439000	0.283981000	3.665320000
H	-3.384114000	0.927136000	2.776313000
H	-3.856642000	0.871017000	4.497522000
H	-4.134793000	-0.535091000	3.436205000
C	0.147485000	-2.051263000	3.162548000
H	-0.300350000	-2.654641000	3.967288000
C	-2.489919000	3.423962000	-1.894924000
H	-3.431919000	3.863523000	-2.263283000
C	-3.941336000	3.510635000	0.655828000
H	-4.186978000	4.365330000	0.004341000
C	-3.056356000	4.015340000	1.816140000
H	-2.806079000	3.192839000	2.500256000
H	-3.594011000	4.782285000	2.393853000
H	-2.114460000	4.454323000	1.462958000
C	0.731560000	-3.003238000	2.104897000
H	-0.033681000	-3.675036000	1.697356000
H	1.519252000	-3.620067000	2.565174000
H	1.167867000	-2.437787000	1.273955000
C	1.245139000	-1.158573000	3.771342000
H	1.710211000	-0.544342000	2.989534000
H	2.029518000	-1.783229000	4.224995000
H	0.857375000	-0.488379000	4.552101000
C	-5.257914000	2.912248000	1.185404000
H	-5.936778000	2.634231000	0.371450000
H	-5.763711000	3.653906000	1.822228000
H	-5.077487000	2.015159000	1.790996000
C	-1.850644000	2.598443000	-3.026089000
H	-0.944303000	2.087996000	-2.666803000
H	-1.568719000	3.260577000	-3.859360000
H	-2.541349000	1.838166000	-3.409915000
C	-1.553815000	4.564819000	-1.454410000
H	-2.015288000	5.220796000	-0.704183000
H	-1.295946000	5.187640000	-2.324320000
H	-0.623848000	4.156755000	-1.037382000
H	-3.758457000	-5.331769000	2.490729000
H	-3.929909000	-3.007018000	-2.057209000
H	-5.556185000	-3.225197000	-1.405573000
H	-6.925609000	0.981651000	-3.183136000
H	0.000452000	-0.844809000	0.001048000

F''(open-shell singlet)

Ti	-1.439749000	0.452111000	0.299951000
P	-1.667168000	-1.016314000	2.372967000
P	-3.168900000	2.322536000	-0.416439000
N	-3.162211000	-0.665864000	-0.158346000
C	-4.150341000	-0.206583000	-1.052851000
C	-5.343308000	1.653552000	-2.136677000
H	-5.467608000	2.726363000	-2.291786000
C	-3.888677000	-4.466450000	1.610757000
C	-3.392641000	-1.944512000	0.399564000
C	-5.007405000	-1.104546000	-1.752461000
C	-4.218781000	-2.907358000	-0.237484000
C	-4.471770000	-4.137731000	0.379795000
H	-5.116828000	-4.857615000	-0.127202000
C	-4.735485000	-2.586205000	-1.621634000
C	-2.792703000	-2.280303000	1.648470000
C	-3.039319000	-3.539347000	2.226897000
H	-2.562413000	-3.799449000	3.171460000
C	-6.021484000	-0.614793000	-2.580200000
H	-6.669446000	-1.328765000	-3.091803000
C	-4.335272000	1.194351000	-1.266334000
C	-2.760819000	-1.358883000	5.083479000
H	-3.327560000	-2.247723000	4.774138000
H	-3.324430000	-0.874015000	5.895655000
H	-1.799353000	-1.685653000	5.500327000
C	-6.202023000	0.761866000	-2.785020000
C	-2.595272000	-0.374294000	3.911831000
H	-1.982615000	0.477886000	4.250487000
C	-3.966687000	0.165051000	3.464702000
H	-3.862382000	0.843810000	2.608204000
H	-4.453557000	0.709199000	4.288085000
H	-4.625616000	-0.658806000	3.157981000
C	-0.279788000	-2.050872000	3.135932000
H	-0.748094000	-2.691554000	3.899116000
C	-2.590857000	3.432448000	-1.838806000
H	-3.498631000	3.870443000	-2.285857000
C	-4.203678000	3.550962000	0.612475000
H	-4.389536000	4.412753000	-0.049421000
C	-3.379425000	4.029183000	1.827302000
H	-3.184523000	3.194986000	2.515273000
H	-3.934546000	4.802779000	2.379118000
H	-2.409698000	4.451522000	1.533241000
C	0.411059000	-2.956984000	2.100692000
H	-0.299457000	-3.646141000	1.627782000
H	1.188476000	-3.555247000	2.601000000
H	0.884109000	-2.360742000	1.311482000
C	0.740920000	-1.127442000	3.828400000
H	1.222849000	-0.473012000	3.089565000
H	1.526726000	-1.727591000	4.311369000
H	0.280247000	-0.493820000	4.599776000
C	-5.563169000	2.981614000	1.058949000
H	-6.195853000	2.714054000	0.205244000
H	-6.093038000	3.735298000	1.661104000
H	-5.439630000	2.083807000	1.677486000
C	-1.868576000	2.586627000	-2.903612000
H	-0.976694000	2.104387000	-2.474203000
H	-1.538294000	3.228974000	-3.734425000
H	-2.523371000	1.807624000	-3.313363000
C	-1.682439000	4.572431000	-1.342611000
H	-2.192501000	5.237643000	-0.633204000
H	-1.358257000	5.185817000	-2.197011000
H	-0.786145000	4.164108000	-0.857483000
H	-4.082384000	-5.432466000	2.075019000
H	-3.970824000	-2.878428000	-2.367759000
H	-5.635176000	-3.173837000	-1.855409000
H	-6.991164000	1.126846000	-3.440691000
H	-0.000131000	1.682524000	-0.000478000
Ti	1.439679000	0.451882000	-0.299491000
P	1.666876000	-1.016323000	-2.372630000
P	3.168804000	2.322476000	0.416516000
N	3.162433000	-0.665838000	0.158321000
C	4.150770000	-0.206457000	1.052586000
C	5.343771000	1.653792000	2.136196000
H	5.467978000	2.726619000	2.291290000
C	3.889382000	-4.466053000	-1.611422000
C	3.393022000	-1.944411000	-0.399799000
C	5.008136000	-1.104335000	1.751920000
C	4.219501000	-2.907138000	0.236969000
C	4.472650000	-4.137372000	-0.380531000
H	5.117963000	-4.857188000	0.126236000
C	4.736374000	-2.586020000	1.621063000

C	2.792890000	-2.280174000	-1.648614000
C	3.039677000	-3.539076000	-2.227270000
H	2.562641000	-3.799164000	-3.171773000
C	6.022371000	-0.614489000	2.579418000
H	6.670566000	-1.328402000	3.090807000
C	4.335588000	1.194498000	1.266072000
C	2.759981000	-1.358142000	-5.083439000
H	3.326995000	-2.246914000	-4.774391000
H	3.323271000	-0.873021000	-5.895687000
H	1.798483000	-1.685064000	-5.500092000
C	6.202773000	0.762184000	2.784266000
C	2.594551000	-0.373791000	-3.911563000
H	1.981671000	0.478359000	-4.249897000
C	3.965981000	0.165694000	-3.464700000
H	3.861784000	0.844214000	-2.608012000
H	4.452498000	0.710156000	-4.288088000
H	4.625169000	-0.658105000	-3.158391000
C	0.279566000	-2.051020000	-3.135467000
H	0.747792000	-2.691507000	-3.898854000
C	2.590732000	3.432085000	1.839090000
H	3.498489000	3.870168000	2.286083000
C	4.203025000	3.551302000	-0.612466000
H	4.388806000	4.413079000	0.049475000
C	3.378359000	4.029491000	-1.827017000
H	3.183371000	3.195345000	-2.515029000
H	3.933241000	4.803223000	-2.378884000
H	2.408661000	4.451661000	-1.532602000
C	-0.410805000	-2.957368000	-2.100105000
H	0.299983000	-3.646460000	-1.627500000
H	-1.188296000	-3.555712000	-2.600203000
H	-0.883678000	-2.361280000	-1.310673000
C	-0.741500000	-1.127662000	-3.827511000
H	-1.223266000	-0.473334000	-3.088473000
H	-1.527381000	-1.727900000	-4.310241000
H	-0.281168000	-0.493930000	-4.599004000
C	5.562589000	2.982372000	-1.059273000
H	6.195540000	2.714984000	-0.205713000
H	6.092121000	3.736230000	-1.661512000
H	5.439232000	2.084545000	-1.677806000
C	1.868745000	2.585943000	2.903832000
H	0.976902000	2.103636000	2.474402000
H	1.538412000	3.228077000	3.734793000
H	2.523687000	1.806968000	3.313393000
C	1.682012000	4.571924000	1.343156000
H	2.191902000	5.237466000	0.633920000
H	1.357620000	5.185019000	2.197685000
H	0.785868000	4.163428000	0.857888000
H	4.083224000	-5.431962000	-2.075854000
H	3.971827000	-2.878344000	2.367262000
H	5.636152000	-3.173572000	1.854688000
H	6.992045000	1.127238000	3.439738000
H	-0.000165000	-0.711429000	0.000370000

F''(triplet)

Ti	1.343291000	0.441676000	-0.251385000
P	1.581331000	-0.634995000	-2.535664000
P	3.132717000	2.158528000	0.742052000
N	3.019699000	-0.757780000	0.058064000
C	4.022271000	-0.467440000	1.004313000
C	5.281505000	1.170393000	2.339711000
H	5.443558000	2.203202000	2.651557000
C	3.560611000	-4.302704000	-2.219766000
C	3.189404000	-1.955512000	-0.671904000
C	4.838067000	-1.490904000	1.566849000
C	3.964313000	-3.035262000	-0.175738000
C	4.155375000	-4.180729000	-0.957095000
H	4.761401000	-4.996125000	-0.558218000
C	4.501918000	-2.927761000	1.233678000
C	2.585510000	-2.073802000	-1.957474000
C	2.769462000	-3.253367000	-2.703464000
H	2.295073000	-3.353586000	-3.678994000
C	5.868710000	-1.164074000	2.452469000
H	6.485798000	-1.968391000	2.856925000
C	4.259639000	0.880927000	1.414085000
C	2.849165000	-0.634756000	-5.198749000
H	3.305424000	-1.614828000	-5.001877000
H	3.523769000	-0.086637000	-5.874868000
H	1.903895000	-0.791454000	-5.734111000
C	6.102676000	0.161564000	2.850414000
C	2.669113000	0.160833000	-3.893216000
H	2.153437000	1.108137000	-4.124141000
C	4.041488000	0.494327000	-3.278839000
H	3.928006000	1.000060000	-2.310868000
H	4.618767000	1.145081000	-3.953016000
H	4.620037000	-0.423336000	-3.105604000
C	0.227615000	-1.470417000	-3.569810000
H	0.748278000	-2.029155000	-4.362549000
C	2.594699000	3.080692000	2.306669000
H	3.516391000	3.454106000	2.783523000
C	4.192770000	3.495454000	-0.114108000
H	4.349274000	4.277070000	0.647042000
C	3.397492000	4.105988000	-1.288170000
H	3.221629000	3.354588000	-2.070172000
H	3.962683000	4.937544000	-1.735601000
H	2.419991000	4.492032000	-0.970192000
C	-0.616036000	-2.465276000	-2.753776000
H	0.003656000	-3.232890000	-2.274651000
H	-1.335675000	-2.966152000	-3.420512000
H	-1.179192000	-1.946647000	-1.967399000
C	-0.674116000	-0.412290000	-4.230874000
H	-1.217897000	0.152574000	-3.462556000
H	-1.416183000	-0.900791000	-4.880249000
H	-0.108546000	0.302998000	-4.844791000
C	5.572005000	2.994161000	-0.580438000
H	6.179036000	2.625581000	0.254069000
H	6.113556000	3.821486000	-1.063849000
H	5.480125000	2.180935000	-1.310828000
C	1.881991000	2.118663000	3.274936000
H	0.982203000	1.693791000	2.804816000
H	1.569663000	2.663307000	4.179394000
H	2.538488000	1.295152000	3.581603000
C	1.688740000	4.279298000	1.968585000
H	2.183912000	5.012341000	1.317395000
H	1.402871000	4.799675000	2.895225000
H	0.770940000	3.934810000	1.474654000
H	3.705724000	-5.203309000	-2.814973000
H	3.730709000	-3.288287000	1.941759000
H	5.377336000	-3.578541000	1.373778000
H	6.902567000	0.397366000	3.550713000
H	-0.017337000	1.567987000	0.359768000
Ti	-1.328732000	0.227148000	0.173959000
P	-1.572297000	-1.212111000	2.236636000
P	-2.902522000	2.328751000	-0.261042000
N	-3.179415000	-0.621189000	-0.201957000
C	-4.154807000	-0.028114000	-1.030615000
C	-5.174260000	1.989631000	-1.985727000
H	-5.192043000	3.074706000	-2.094967000
C	-4.177567000	-4.396885000	1.475498000
C	-3.499121000	-1.894242000	0.329687000
C	-5.126805000	-0.807016000	-1.715414000
C	-4.453090000	-2.739034000	-0.294108000
C	-4.794858000	-3.962194000	0.295427000
H	-5.539568000	-4.592331000	-0.193987000
C	-5.012606000	-2.313859000	-1.635193000
C	-2.858276000	-2.336674000	1.524289000
C	-3.201051000	-3.587335000	2.069863000
H	-2.699200000	-3.934720000	2.972478000
C	-6.110555000	-0.177685000	-2.485388000

H	-6.852993000	-0.794962000	-2.994185000
C	-4.192934000	1.391290000	-1.173507000
C	-2.440266000	-1.556790000	5.029288000
H	-3.037140000	-2.441783000	4.768509000
H	-2.933107000	-1.068941000	5.884635000
H	-1.450572000	-1.890596000	5.365868000
C	-6.143004000	1.216998000	-2.635132000
C	-2.367033000	-0.569955000	3.849898000
H	-1.723146000	0.277594000	4.135071000
C	-3.770126000	-0.027816000	3.520432000
H	-3.747168000	0.608491000	2.626877000
H	-4.162590000	0.561941000	4.362384000
H	-4.466371000	-0.854008000	3.322909000
C	-0.260056000	-2.422787000	2.863754000
H	-0.747640000	-3.058741000	3.618925000
C	-2.342631000	3.616359000	-1.532918000
H	-3.243053000	4.185349000	-1.818814000
C	-3.817429000	3.470235000	0.972056000
H	-3.929093000	4.432296000	0.445568000
C	-2.942508000	3.695102000	2.223186000
H	-2.798366000	2.755959000	2.772714000
H	-3.428808000	4.417427000	2.896518000
H	-1.947675000	4.082244000	1.968434000
C	0.274526000	-3.322735000	1.734732000
H	-0.524738000	-3.921719000	1.280394000
H	1.029310000	-4.012968000	2.142615000
H	0.743211000	-2.720229000	0.947104000
C	0.887614000	-1.646031000	3.536070000
H	1.396112000	-1.011192000	2.798149000
H	1.627700000	-2.348615000	3.948246000
H	0.538448000	-1.004101000	4.357367000
C	-5.222825000	2.970153000	1.353957000
H	-5.885281000	2.907938000	0.483099000
H	-5.670475000	3.665560000	2.080343000
H	-5.188177000	1.976965000	1.818250000
C	-1.761178000	2.937200000	-2.783435000
H	-0.881357000	2.332764000	-2.515503000
H	-1.443975000	3.698875000	-3.512265000
H	-2.496416000	2.283795000	-3.269463000
C	-1.316331000	4.590993000	-0.924574000
H	-1.721056000	5.150446000	-0.070859000
H	-1.007147000	5.324144000	-1.684968000
H	-0.424538000	4.044213000	-0.591478000
H	-4.442142000	-5.356949000	1.916559000
H	-4.332790000	-2.666070000	-2.435340000
H	-5.984794000	-2.791391000	-1.825587000
H	-6.908691000	1.689637000	-3.248531000
H	0.077980000	-0.885553000	-0.230876000

F''(quintet)

Ti	1.455400000	0.477563000	-0.335919000
P	1.806086000	-0.982168000	-2.406198000
P	3.191367000	2.308135000	0.417338000
N	3.117326000	-0.675230000	0.219648000
C	4.075455000	-0.230048000	1.151370000
C	5.257745000	1.617344000	2.263382000
H	5.401848000	2.688688000	2.410469000
C	3.790928000	-4.525197000	-1.457040000
C	3.336090000	-1.966347000	-0.310767000
C	4.874336000	-1.139205000	1.901266000
C	4.097025000	-2.945898000	0.379612000
C	4.328537000	-4.196222000	-0.205163000
H	4.921531000	-4.930936000	0.342457000
C	4.572255000	-2.616336000	1.777194000
C	2.794094000	-2.297259000	-1.587122000
C	3.016469000	-3.574959000	-2.133418000
H	2.582552000	-3.829974000	-3.100029000
C	5.857615000	-0.661184000	2.772499000
H	6.462360000	-1.381775000	3.325967000
C	4.283936000	1.169614000	1.348630000
C	3.071987000	-1.379065000	-5.028866000
H	3.524884000	-2.321824000	-4.692253000
H	3.744832000	-0.940120000	-5.781764000
H	2.122250000	-1.607558000	-5.529545000
C	6.059226000	0.714157000	2.967091000
C	2.903508000	-0.398056000	-3.854397000
H	2.396570000	0.510158000	-4.220676000
C	4.278768000	0.007469000	-3.292091000
H	4.170439000	0.658315000	-2.414910000
H	4.864367000	0.539689000	-4.056701000
H	4.845129000	-0.880189000	-2.979316000
C	0.427427000	-1.924540000	-3.288777000
H	0.916772000	-2.596794000	-4.010463000
C	2.594449000	3.481640000	1.783294000
H	3.500558000	3.909943000	2.242958000
C	4.305648000	3.494374000	-0.586650000
H	4.443295000	4.384242000	0.049113000
C	3.567140000	3.917345000	-1.874389000
H	3.411487000	3.051786000	-2.533331000
H	4.160540000	4.662949000	-2.425067000
H	2.582625000	4.355448000	-1.662908000
C	-0.407893000	-2.778925000	-2.318100000
H	0.213405000	-3.504780000	-1.779112000
H	-1.170096000	-3.334307000	-2.886637000
H	-0.914924000	-2.150600000	-1.576215000
C	-0.465811000	-0.936569000	-4.065029000
H	-0.963932000	-0.245467000	-3.371758000
H	-1.246414000	-1.484583000	-4.613619000
H	0.101310000	-0.340728000	-4.794423000
C	5.694655000	2.914643000	-0.910508000
H	6.264711000	2.683516000	-0.003621000
H	6.265866000	3.646685000	-1.501702000
H	5.619225000	1.992930000	-1.500620000
C	1.813196000	2.701897000	2.855788000
H	0.918936000	2.234211000	2.416492000
H	1.481390000	3.385847000	3.652113000
H	2.428534000	1.917061000	3.313034000
C	1.739375000	4.628202000	1.213744000
H	2.290516000	5.246301000	0.492455000
H	1.409205000	5.287499000	2.030852000
H	0.845494000	4.227689000	0.718362000
H	3.966328000	-5.507379000	-1.893796000
H	3.776954000	-2.882222000	2.500168000
H	5.449899000	-3.220974000	2.048791000
H	6.822998000	1.070304000	3.656875000
H	0.000211000	1.700523000	0.000761000
Ti	-1.455111000	0.477347000	0.336414000
P	-1.807238000	-0.983039000	2.405910000
P	-3.189763000	2.309195000	-0.416367000
N	-3.117701000	-0.674209000	-0.219975000
C	-4.075286000	-0.228044000	-1.151765000
C	-5.255857000	1.620621000	-2.263545000
H	-5.399105000	2.692125000	-2.410302000
C	-3.793345000	-4.524761000	1.454587000
C	-3.337286000	-1.965465000	0.309755000
C	-4.874610000	-1.136345000	-1.902215000
C	-4.098682000	-2.944257000	-0.381186000
C	-4.330748000	-4.194819000	0.202879000
H	-4.924056000	-4.928958000	-0.345176000
C	-4.573826000	-2.613789000	-1.778588000
C	-2.795593000	-2.297326000	1.586000000
C	-3.018554000	-3.575226000	2.131577000
H	-2.584836000	-3.830935000	3.098096000
C	-5.857193000	-0.657284000	-2.773670000
H	-6.462272000	-1.377244000	-3.327595000
C	-4.282735000	1.171851000	-1.348577000
C	-3.073436000	-1.380610000	5.028352000
H	-3.526222000	-2.323315000	4.691436000

H	-3.746438000	-0.941891000	5.781242000
H	-2.123770000	-1.609167000	5.529137000
C	-6.057707000	0.718265000	-2.967903000
C	-2.904816000	-0.399292000	3.854156000
H	-2.397924000	0.508823000	4.220743000
C	-4.280039000	0.006358000	3.291827000
H	-4.171671000	0.657295000	2.414720000
H	-4.865645000	0.538511000	4.056476000
H	-4.846409000	-0.881252000	2.978937000
C	-0.429027000	-1.926210000	3.288331000
H	-0.918644000	-2.598552000	4.009752000
C	-2.591929000	3.483496000	-1.781195000
H	-3.497640000	3.913126000	-2.240406000
C	-4.303439000	3.495230000	0.588536000
H	-4.440038000	4.385999000	-0.046192000
C	-3.565071000	3.916017000	1.877082000
H	-3.410450000	3.049529000	2.535044000
H	-4.158015000	4.661506000	2.428406000
H	-2.580077000	4.353477000	1.666488000
C	0.406201000	-2.780545000	2.317537000
H	-0.215232000	-3.506038000	1.778212000
H	1.168109000	-3.336354000	2.886056000
H	0.913557000	-2.152141000	1.575945000
C	0.464351000	-0.938670000	4.064993000
H	0.962687000	-0.247471000	3.371970000
H	1.244782000	-1.486994000	4.613521000
H	-0.102731000	-0.342920000	4.794491000
C	-5.693088000	2.916329000	0.911092000
H	-6.263017000	2.686962000	0.003677000
H	-6.263871000	3.648068000	1.503077000
H	-5.618727000	1.993728000	1.499956000
C	-1.811355000	2.704197000	-2.854496000
H	-0.917542000	2.235248000	-2.415639000
H	-1.478888000	3.388696000	-3.650077000
H	-2.427369000	1.920397000	-3.312601000
C	-1.735791000	4.628633000	-1.210373000
H	-2.286319000	5.246393000	-0.488323000
H	-1.405042000	5.288587000	-2.026717000
H	-0.842292000	4.226640000	-0.715499000
H	-3.969179000	-5.507130000	1.890748000
H	-3.778955000	-2.880255000	-2.501824000
H	-5.452104000	-3.217519000	-2.050178000
H	-6.820931000	1.075202000	-3.657883000
H	0.000304000	-0.690917000	0.000564000

$TS_{F''G}$ (closed-shell singlet)

Ti	-1.229401000	0.474372000	0.507320000
P	-1.433284000	-1.056691000	2.515128000
P	-2.490592000	2.299910000	-0.885071000
N	-3.004137000	-0.577358000	-0.057628000
C	-3.866140000	-0.134126000	-1.084853000
C	-4.684698000	1.677665000	-2.551637000
H	-4.593654000	2.706139000	-2.905595000
C	-4.058328000	-4.208305000	1.946993000
C	-3.346824000	-1.793985000	0.578357000
C	-4.861103000	-0.970991000	-1.671832000
C	-4.310050000	-2.695823000	0.045080000
C	-4.668272000	-3.858408000	0.737241000
H	-5.420128000	-4.515037000	0.295499000
C	-4.875656000	-2.440313000	-1.330416000
C	-2.723100000	-2.158904000	1.815334000
C	-3.073594000	-3.360888000	2.461534000
H	-2.567522000	-3.634274000	3.386535000
C	-5.758712000	-0.464959000	-2.617542000
H	-6.513895000	-1.139505000	-3.025481000
C	-3.778877000	1.204401000	-1.584688000
C	-2.365155000	-1.280454000	5.301293000
H	-3.006031000	-2.139284000	5.060228000
H	-2.838062000	-0.741546000	6.136984000
H	-1.397264000	-1.655433000	5.657578000
C	-5.693528000	0.860442000	-3.067023000
C	-2.228389000	-0.332793000	4.095138000
H	-1.552737000	0.490833000	4.376622000
C	-3.601645000	0.264497000	3.731202000
H	-3.542844000	0.915218000	2.849691000
H	-3.997009000	0.855009000	4.571575000
H	-4.320103000	-0.533963000	3.502524000
C	-0.126838000	-2.232304000	3.206898000
H	-0.610248000	-2.830192000	3.994963000
C	-1.740741000	3.235760000	-2.357483000
H	-2.471022000	4.013846000	-2.636883000
C	-3.603542000	3.650939000	-0.127569000
H	-4.293432000	3.914620000	-0.945786000
C	-2.856560000	4.925634000	0.306694000
H	-2.053281000	4.701357000	1.021388000
H	-3.561540000	5.611889000	0.800170000
H	-2.420402000	5.460597000	-0.545884000
C	0.399858000	-3.183691000	2.119291000
H	-0.401648000	-3.810502000	1.709364000
H	1.166655000	-3.846056000	2.549892000
H	0.847563000	-2.618566000	1.293566000
C	1.015675000	-1.412334000	3.838708000
H	1.508071000	-0.794308000	3.075959000
H	1.769515000	-2.087549000	4.270952000
H	0.661068000	-0.749857000	4.641626000
C	-4.436455000	3.077715000	1.033036000
H	-4.951462000	2.152012000	0.747338000
H	-5.195726000	3.811155000	1.343824000
H	-3.802416000	2.868153000	1.904095000
C	-1.485113000	2.325285000	-3.570265000
H	-0.769765000	1.536671000	-3.299720000
H	-1.048678000	2.920266000	-4.387299000
H	-2.399625000	1.847299000	-3.938583000
C	-0.415876000	3.905632000	-1.943040000
H	-0.524146000	4.588799000	-1.093417000
H	-0.008789000	4.476794000	-2.791348000
H	0.316435000	3.137276000	-1.658049000
H	-4.334324000	-5.123506000	2.468731000
H	-4.267382000	-2.987276000	-2.076761000
H	-5.893782000	-2.849810000	-1.414664000
H	-6.395575000	1.236010000	-3.809710000
H	0.187293000	1.679331000	0.528512000
Ti	1.191086000	0.361312000	-0.320820000
P	1.164705000	-1.162851000	-2.390662000
P	3.152299000	2.120701000	0.211593000
N	2.813890000	-0.901323000	0.074018000
C	3.894233000	-0.497262000	0.889154000
C	5.319172000	1.270656000	1.836515000
H	5.548280000	2.331276000	1.949245000
C	3.243215000	-4.723796000	-1.729934000
C	2.938235000	-2.190254000	-0.491674000
C	4.718793000	-1.450478000	1.556244000
C	3.735104000	-3.199869000	0.107229000
C	3.894679000	-4.439166000	-0.522891000
H	4.517589000	-5.197471000	-0.045389000
C	4.329299000	-2.907582000	1.465030000
C	2.269252000	-2.477978000	-1.714732000
C	2.420909000	-3.747904000	-2.305148000
H	1.894444000	-3.978857000	-3.230025000
C	5.824178000	-1.035742000	2.302854000
H	6.441530000	-1.793807000	2.787903000
C	4.218059000	0.884889000	1.044645000
C	2.089043000	-1.611308000	-5.159305000
H	2.653553000	-2.506605000	-4.865150000
H	2.612548000	-1.158404000	-6.015753000
H	1.096492000	-1.923209000	-5.508853000
C	6.136261000	0.323837000	2.457233000
C	2.020559000	-0.596773000	-4.003631000

H	1.413822000	0.265477000	-4.327792000
C	3.429484000	-0.088167000	-3.651010000
H	3.391174000	0.609494000	-2.803509000
H	3.883182000	0.426507000	-4.511594000
H	4.082641000	-0.924120000	-3.364451000
C	-0.276774000	-2.197628000	-3.056662000
H	0.170173000	-2.879082000	-3.797042000
C	2.840835000	3.354236000	1.622820000
H	3.824680000	3.771853000	1.894858000
C	4.305434000	3.157342000	-0.908449000
H	4.656837000	3.986942000	-0.273077000
C	3.515457000	3.750608000	-2.093629000
H	3.131069000	2.954377000	-2.745372000
H	4.173728000	4.394034000	-2.696813000
H	2.661511000	4.355617000	-1.764720000
C	-0.937469000	-3.046573000	-1.957195000
H	-0.217928000	-3.720196000	-1.476202000
H	-1.735540000	-3.660539000	-2.403565000
H	-1.376592000	-2.406082000	-1.185237000
C	-1.317787000	-1.321987000	-3.775365000
H	-1.798866000	-0.637276000	-3.066741000
H	-2.100907000	-1.959524000	-4.213296000
H	-0.878534000	-0.727800000	-4.589266000
C	5.535269000	2.375454000	-1.407447000
H	6.164178000	2.028213000	-0.580301000
H	6.141264000	3.028971000	-2.053393000
H	5.242615000	1.497921000	-1.996965000
C	2.250927000	2.634070000	2.849709000
H	1.309061000	2.133488000	2.585413000
H	2.041943000	3.365310000	3.645754000
H	2.942402000	1.881965000	3.247930000
C	1.924783000	4.506443000	1.171378000
H	2.355183000	5.082521000	0.341204000
H	1.762480000	5.202924000	2.008140000
H	0.948786000	4.114552000	0.856456000
H	3.365098000	-5.694105000	-2.209586000
H	3.576608000	-3.130476000	2.245115000
H	5.191700000	-3.558264000	1.669702000
H	6.994830000	0.633403000	3.051267000
H	-0.144371000	-0.864921000	-0.031220000
N	-1.220607000	3.851547000	4.187442000
N	-1.354812000	3.118509000	3.357442000

$TS_{F''G}$ (open-shell singlet)

Ti	-1.435657000	0.486008000	0.196849000
P	-1.768595000	-0.475627000	2.544595000
P	-3.154453000	1.994366000	-1.179114000
N	-3.034656000	-0.846994000	-0.109103000
C	-3.986650000	-0.687698000	-1.136405000
C	-5.223843000	0.767450000	-2.689133000
H	-5.387774000	1.755718000	-3.121691000
C	-3.463617000	-4.277572000	2.380973000
C	-3.180421000	-2.001286000	0.696012000
C	-4.752123000	-1.783661000	-1.632237000
C	-3.881886000	-3.153560000	0.254182000
C	-4.028423000	-4.259923000	1.099583000
H	-4.576618000	-5.130070000	0.733832000
C	-4.391213000	-3.176322000	-1.168125000
C	-2.620588000	-2.013243000	2.008183000
C	-2.755389000	-3.153123000	2.821553000
H	-2.307614000	-3.160188000	3.814973000
C	-5.755897000	-1.576379000	-2.582599000
H	-6.334513000	-2.435734000	-2.926400000
C	-4.228949000	0.600875000	-1.706327000
C	-3.109115000	-0.385567000	5.162975000
H	-3.401759000	-1.440475000	5.067578000
H	-3.884368000	0.117982000	5.761183000
H	-2.170779000	-0.333406000	5.730020000
C	-6.009170000	-0.305311000	-3.118983000
C	-3.011219000	0.288029000	3.781668000
H	-2.654288000	1.320648000	3.919407000
C	-4.401701000	0.337123000	3.118159000
H	-4.346871000	0.719277000	2.091988000
H	-5.077699000	0.983340000	3.698384000
H	-4.840807000	-0.668527000	3.075191000
C	-0.381438000	-1.072919000	3.681131000
H	-0.864995000	-1.601095000	4.517153000
C	-2.444874000	2.631838000	-2.826326000
H	-3.270165000	3.139629000	-3.353274000
C	-4.443723000	3.324931000	-0.748491000
H	-5.119935000	3.352769000	-1.618069000
C	-3.857607000	4.735270000	-0.546110000
H	-3.056072000	4.736586000	0.205035000
H	-4.650729000	5.410190000	-0.190278000
H	-3.461368000	5.157227000	-1.477254000
C	0.581958000	-2.050316000	2.984879000
H	0.055695000	-2.927384000	2.588859000
H	1.334126000	-2.397552000	3.710682000
H	1.102183000	-1.565475000	2.150023000
C	0.380286000	0.142792000	4.246731000
H	0.871518000	0.696929000	3.435522000
H	1.159449000	-0.192349000	4.947627000
H	-0.278642000	0.838767000	4.785425000
C	-5.260461000	2.894811000	0.482861000
H	-5.683498000	1.890214000	0.358991000
H	-6.090651000	3.599674000	0.640589000
H	-4.637337000	2.900166000	1.386814000
C	-1.937721000	1.462560000	-3.693509000
H	-1.130432000	0.923695000	-3.174459000
H	-1.522837000	1.855666000	-4.634392000
H	-2.731458000	0.747231000	-3.936713000
C	-1.285133000	3.625018000	-2.602016000
H	-1.560784000	4.483141000	-1.978664000
H	-0.940422000	4.011432000	-3.573681000
H	-0.446974000	3.109899000	-2.115617000
H	-3.570890000	-5.150975000	3.022743000
H	-3.599403000	-3.579245000	-1.829266000
H	-5.249057000	-3.857585000	-1.268483000
H	-6.789029000	-0.161239000	-3.865232000
H	0.030254000	1.560047000	-0.401537000
Ti	1.463592000	0.290050000	-0.371569000
P	1.708681000	-1.692359000	-1.969335000
P	3.179863000	2.313423000	-0.288767000
N	3.229457000	-0.620806000	0.328215000
C	4.233322000	0.090822000	1.017545000
C	5.423271000	2.196280000	1.469764000
H	5.531948000	3.268770000	1.301534000
C	4.066506000	-4.735290000	-0.353692000
C	3.493114000	-1.997763000	0.137232000
C	5.127062000	-0.556289000	1.919139000
C	4.357947000	-2.724331000	0.996877000
C	4.648042000	-4.067668000	0.732392000
H	5.322486000	-4.602505000	1.403485000
C	4.879316000	-2.015850000	2.226488000
C	2.892188000	-2.677725000	-0.960588000
C	3.179174000	-4.037492000	-1.182211000
H	2.703506000	-4.559260000	-2.012164000
C	6.155987000	0.162602000	2.533565000
H	6.832027000	-0.364727000	3.208937000
C	4.398864000	1.493491000	0.805123000
C	2.753971000	-2.704004000	-4.526426000
H	3.342859000	-3.475496000	-4.011577000
H	3.294048000	-2.436916000	-5.448050000
H	1.791513000	-3.139955000	-4.823740000
C	6.316613000	1.540688000	2.321096000
C	2.590807000	-1.453351000	-3.644077000
H	1.953513000	-0.726788000	-4.175125000
C	3.959053000	-0.796521000	-3.383293000

H	3.858673000	0.068339000	-2.714558000
H	4.412345000	-0.461321000	-4.328399000
H	4.645007000	-1.508600000	-2.904473000
C	0.359438000	-2.947943000	-2.385079000
H	0.843716000	-3.753023000	-2.959355000
C	2.623978000	3.767204000	0.791333000
H	3.535816000	4.330178000	1.050945000
C	4.147123000	3.229350000	-1.655283000
H	4.313167000	4.247867000	-1.267623000
C	3.279134000	3.322662000	-2.928576000
H	3.098604000	2.323817000	-3.348937000
H	3.793546000	3.925402000	-3.692279000
H	2.302079000	3.783504000	-2.733422000
C	-0.261392000	-3.558096000	-1.115543000
H	0.487161000	-4.090661000	-0.516008000
H	-1.046961000	-4.275627000	-1.398005000
H	-0.710496000	-2.779199000	-0.488608000
C	-0.718752000	-2.293933000	-3.269889000
H	-1.240969000	-1.504973000	-2.712892000
H	-1.465431000	-3.044550000	-3.570206000
H	-0.301467000	-1.852135000	-4.186213000
C	5.518719000	2.602197000	-1.966952000
H	6.177441000	2.599322000	-1.091309000
H	6.007913000	3.178477000	-2.766972000
H	5.418841000	1.566004000	-2.313129000
C	1.980635000	3.235634000	2.084589000
H	1.083935000	2.642342000	1.849839000
H	1.671353000	4.075091000	2.725717000
H	2.676983000	2.608298000	2.654981000
C	1.656667000	4.704254000	0.044817000
H	2.109748000	5.143951000	-0.853859000
H	1.361990000	5.533752000	0.705602000
H	0.747795000	4.164031000	-0.249766000
H	4.290231000	-5.784292000	-0.542915000
H	4.124236000	-2.091044000	3.033131000
H	5.790343000	-2.499105000	2.607959000
H	7.117758000	2.088651000	2.814820000
H	0.006734000	-0.715710000	0.275394000
N	-1.793062000	4.206111000	3.601903000
N	-1.625404000	3.844887000	2.560625000

$TS_{F''G}$ (triplet)

Ti	1.404912000	-0.493582000	0.025940000
P	2.011496000	-0.570979000	2.538404000
P	3.034874000	-1.222167000	-1.896301000
N	2.866583000	0.959465000	0.175486000
C	3.766935000	1.276958000	-0.865253000
C	4.993826000	0.604001000	-2.882604000
H	5.191155000	-0.134079000	-3.661415000
C	3.089493000	3.275691000	3.737302000
C	2.970918000	1.744491000	1.348805000
C	4.430197000	2.534182000	-0.926286000
C	3.532335000	3.045682000	1.346666000
C	3.590566000	3.787209000	2.534611000
H	4.022169000	4.789366000	2.506829000
C	4.008546000	3.625530000	0.033820000
C	2.521823000	1.196580000	2.586860000
C	2.563555000	1.976936000	3.755509000
H	2.199007000	1.563713000	4.695395000
C	5.392183000	2.773690000	-1.914444000
H	5.898913000	3.740406000	-1.927328000
C	4.042721000	0.318262000	-1.885964000
C	3.815982000	-1.252487000	4.757106000
H	3.910103000	-0.188364000	5.015368000
H	4.762569000	-1.742987000	5.032300000
H	3.025445000	-1.693570000	5.377510000
C	5.692102000	1.816239000	-2.893293000
C	3.570179000	-1.429780000	3.246782000
H	3.413184000	-2.498552000	3.032838000
C	4.807651000	-0.951121000	2.461818000
H	4.625269000	-0.942773000	1.381488000
H	5.664154000	-1.610169000	2.669031000
H	5.079936000	0.069134000	2.763214000
C	0.789357000	-0.753486000	3.970682000
H	1.313710000	-0.388101000	4.866895000
C	2.293074000	-1.231449000	-3.653626000
H	3.113708000	-1.499674000	-4.340460000
C	4.386952000	-2.556407000	-2.066488000
H	4.995994000	-2.238917000	-2.928540000
C	3.835591000	-3.965674000	-2.356323000
H	3.083147000	-4.264082000	-1.613353000
H	4.657491000	-4.696427000	-2.311986000
H	3.385499000	-4.038318000	-3.353373000
C	-0.486319000	0.088241000	3.788253000
H	-0.255526000	1.145626000	3.610161000
H	-1.106523000	0.013236000	4.695223000
H	-1.077434000	-0.269306000	2.935540000
C	0.440567000	-2.239337000	4.194766000
H	-0.082881000	-2.652054000	3.323498000
H	-0.225272000	-2.339739000	5.064961000
H	1.329786000	-2.856739000	4.381036000
C	5.286809000	-2.574200000	-0.819772000
H	5.718187000	-1.585963000	-0.618932000
H	6.113459000	-3.285614000	-0.968597000
H	4.721278000	-2.891473000	0.066572000
C	1.742908000	0.155427000	-4.039452000
H	0.941555000	0.448220000	-3.346511000
H	1.313864000	0.109663000	-5.052640000
H	2.517491000	0.930696000	-4.027213000
C	1.155809000	-2.266924000	-3.775275000
H	1.464820000	-3.285904000	-3.514808000
H	0.782238000	-2.283184000	-4.811014000
H	0.329447000	-1.979495000	-3.112791000
H	3.123435000	3.870368000	4.649184000
H	3.189034000	4.210181000	-0.426233000
H	4.831367000	4.337169000	0.199360000
H	6.440763000	2.019558000	-3.657674000
H	-0.012612000	-0.801233000	-1.181622000
Ti	-1.485303000	-0.084070000	-0.182742000
P	-1.833276000	2.217175000	-1.297173000
P	-2.907764000	-2.220160000	-0.775485000
N	-3.382801000	0.425390000	0.510680000
C	-4.291382000	-0.549933000	0.975622000
C	-5.153623000	-2.846418000	0.892312000
H	-5.102193000	-3.857666000	0.486852000
C	-4.678339000	4.467361000	0.773187000
C	-3.798413000	1.771447000	0.633554000
C	-5.290861000	-0.246003000	1.940119000
C	-4.791471000	2.163149000	1.569956000
C	-5.234099000	3.490291000	1.609294000
H	-6.008448000	3.764740000	2.327834000
C	-5.276182000	1.131253000	2.564820000
C	-3.215832000	2.767240000	-0.205135000
C	-3.656867000	4.100288000	-0.111421000
H	-3.195299000	4.864194000	-0.735984000
C	-6.211830000	-1.224238000	2.329147000
H	-6.977202000	-0.961985000	3.061643000
C	-4.231852000	-1.876841000	0.454951000
C	-2.731126000	3.847070000	-3.559276000
H	-3.507900000	4.340601000	-2.959897000
H	-3.083110000	3.825404000	-4.602120000
H	-1.823284000	4.463091000	-3.530251000
C	-6.153531000	-2.528829000	1.817644000
C	-2.488487000	2.406938000	-3.072004000
H	-1.697390000	1.950668000	-3.688400000
C	-3.767129000	1.563657000	-3.221119000
H	-3.603569000	0.538824000	-2.866564000
H	-4.079250000	1.523882000	-4.275424000

H	-4.588848000	1.996787000	-2.634269000
C	-0.594918000	3.629922000	-1.129616000
H	-1.114931000	4.555159000	-1.423046000
C	-2.249803000	-3.893623000	-0.185076000
H	-3.112958000	-4.576942000	-0.130850000
C	-3.817395000	-2.737972000	-2.374556000
H	-3.958549000	-3.828069000	-2.286820000
C	-2.939494000	-2.452907000	-3.610254000
H	-2.760114000	-1.375883000	-3.722539000
H	-3.446010000	-2.812964000	-4.518671000
H	-1.961303000	-2.944392000	-3.549201000
C	-0.131151000	3.767311000	0.332910000
H	-0.971696000	3.995244000	1.000948000
H	0.601974000	4.583574000	0.416287000
H	0.345841000	2.841649000	0.680035000
C	0.598591000	3.409970000	-2.077803000
H	1.151751000	2.504835000	-1.796250000
H	1.289298000	4.263897000	-2.012114000
H	0.289576000	3.313033000	-3.127968000
C	-5.204833000	-2.083679000	-2.516975000
H	-5.878842000	-2.374476000	-1.703401000
H	-5.657119000	-2.395753000	-3.470614000
H	-5.136920000	-0.988590000	-2.520015000
C	-1.642799000	-3.740736000	1.219318000
H	-0.800495000	-3.031628000	1.191649000
H	-1.258312000	-4.707884000	1.576521000
H	-2.381447000	-3.374821000	1.944026000
C	-1.217499000	-4.479726000	-1.166876000
H	-1.653873000	-4.690676000	-2.151945000
H	-0.825267000	-5.427397000	-0.768251000
H	-0.372196000	-3.791621000	-1.300553000
H	-5.020980000	5.499845000	0.823826000
H	-4.591650000	1.124620000	3.435860000
H	-6.269093000	1.396119000	2.956336000
H	-6.872115000	-3.281949000	2.137550000
H	-0.015200000	0.366260000	0.883839000
N	2.575944000	-5.111622000	1.822528000
N	2.005593000	-4.536020000	1.055087000

$TS_{F''G}$ (quintet)

Ti	-1.446698000	0.506912000	0.175189000
P	-1.906769000	-0.317194000	2.562624000
P	-3.149807000	1.893125000	-1.306200000
N	-2.983940000	-0.888258000	-0.126939000
C	-3.918117000	-0.801306000	-1.177284000
C	-5.171757000	0.556918000	-2.798346000
H	-5.361051000	1.522639000	-3.269581000
C	-3.351573000	-4.222087000	2.495182000
C	-3.116502000	-2.008010000	0.725164000
C	-4.636417000	-1.940229000	-1.642576000
C	-3.755324000	-3.206101000	0.311136000
C	-3.876491000	-4.282898000	1.197572000
H	-4.373923000	-5.191658000	0.853895000
C	-4.232383000	-3.300758000	-1.120081000
C	-2.612592000	-1.934608000	2.057730000
C	-2.719359000	-3.045358000	2.914335000
H	-2.313288000	-2.987050000	3.923945000
C	-5.630025000	-1.800458000	-2.615993000
H	-6.174480000	-2.689510000	-2.939367000
C	-4.187725000	0.458220000	-1.795310000
C	-3.406879000	-0.193728000	5.086411000
H	-3.605103000	-1.273400000	5.034472000
H	-4.256742000	0.272058000	5.608952000
H	-2.513120000	-0.031990000	5.702625000
C	-5.914666000	-0.556781000	-3.199779000
C	-3.279899000	0.411869000	3.676232000
H	-3.016028000	1.476716000	3.771736000
C	-4.627163000	0.306746000	2.934021000
H	-4.540501000	0.626896000	1.889184000
H	-5.383613000	0.932185000	3.431563000
H	-4.984526000	-0.731541000	2.936237000
C	-0.550528000	-0.740407000	3.807365000
H	-1.038607000	-1.270970000	4.639339000
C	-2.434256000	2.481942000	-2.973368000
H	-3.262645000	2.969908000	-3.514170000
C	-4.469514000	3.224882000	-0.967560000
H	-5.123352000	3.211504000	-1.854461000
C	-3.898713000	4.646834000	-0.807705000
H	-3.111707000	4.681913000	-0.041852000
H	-4.702363000	5.329854000	-0.493116000
H	-3.486226000	5.035981000	-1.746132000
C	0.531009000	-1.661489000	3.214993000
H	0.103716000	-2.595124000	2.829309000
H	1.262370000	-1.913329000	3.999069000
H	1.061754000	-1.172245000	2.389266000
C	0.071200000	0.560450000	4.355776000
H	0.561579000	1.122182000	3.549208000
H	0.833305000	0.324016000	5.113264000
H	-0.674765000	1.217579000	4.824895000
C	-5.312174000	2.836966000	0.259487000
H	-5.736514000	1.830531000	0.157266000
H	-6.142641000	3.549029000	0.379939000
H	-4.706458000	2.866221000	1.175135000
C	-1.919415000	1.294761000	-3.810237000
H	-1.111314000	0.773085000	-3.275914000
H	-1.504626000	1.666689000	-4.759832000
H	-2.708542000	0.569142000	-4.037196000
C	-1.281763000	3.488629000	-2.777583000
H	-1.561095000	4.358908000	-2.172818000
H	-0.942207000	3.854987000	-3.758887000
H	-0.438715000	2.990430000	-2.282190000
H	-3.436775000	-5.074302000	3.167978000
H	-3.412030000	-3.695649000	-1.750327000
H	-5.061111000	-4.018303000	-1.211568000
H	-6.687294000	-0.464537000	-3.961707000
H	0.030008000	1.528268000	-0.512948000
Ti	1.480304000	0.265629000	-0.425607000
P	1.851967000	-1.796434000	-1.897588000
P	3.157938000	2.309772000	-0.391428000
N	3.216105000	-0.572086000	0.416331000
C	4.183948000	0.193411000	1.098277000
C	5.335252000	2.336724000	1.454359000
H	5.441858000	3.396875000	1.220080000
C	4.113781000	-4.713693000	0.045122000
C	3.501501000	-1.954573000	0.325718000
C	5.043079000	-0.382834000	2.077106000
C	4.328221000	-2.614943000	1.272223000
C	4.637387000	-3.970230000	1.111712000
H	5.281239000	-4.453740000	1.848531000
C	4.790984000	-1.820439000	2.472448000
C	2.965358000	-2.709828000	-0.756063000
C	3.269026000	-4.079019000	-0.873331000
H	2.840319000	-4.656597000	-1.691856000
C	6.040109000	0.386675000	2.683161000
H	6.691318000	-0.085930000	3.420532000
C	4.344790000	1.579763000	0.797189000
C	3.037443000	-2.959152000	-4.322386000
H	3.584990000	-3.703978000	-3.728620000
H	3.635865000	-2.750474000	-5.222714000
H	2.090016000	-3.403992000	-4.652864000
C	6.197949000	1.748829000	2.383286000
C	2.835286000	-1.657460000	-3.525841000
H	2.238725000	-0.958738000	-4.135564000
C	4.192405000	-0.996409000	-3.220676000
H	4.062514000	-0.094114000	-2.609038000
H	4.703496000	-0.718900000	-4.154817000
H	4.841523000	-1.685280000	-2.663226000
C	0.518633000	-3.066634000	-2.315687000

H	1.026654000	-3.907204000	-2.813539000
C	2.551434000	3.823010000	0.577519000
H	3.451906000	4.409241000	0.825114000
C	4.159793000	3.162318000	-1.776925000
H	4.277401000	4.210648000	-1.457196000
C	3.343477000	3.135491000	-3.086814000
H	3.205581000	2.102737000	-3.436226000
H	3.872174000	3.693819000	-3.874174000
H	2.347597000	3.581300000	-2.964489000
C	-0.175952000	-3.596043000	-1.048041000
H	0.535576000	-4.085489000	-0.371705000
H	-0.942433000	-4.333932000	-1.330094000
H	-0.661879000	-2.781008000	-0.499388000
C	-0.503781000	-2.459490000	-3.295826000
H	-1.046678000	-1.633068000	-2.818436000
H	-1.241896000	-3.221203000	-3.588971000
H	-0.033453000	-2.079305000	-4.214106000
C	5.561999000	2.561764000	-1.986958000
H	6.182504000	2.642151000	-1.087357000
H	6.067552000	3.096471000	-2.805527000
H	5.509335000	1.501044000	-2.261845000
C	1.875744000	3.373754000	1.885143000
H	0.986746000	2.763871000	1.665599000
H	1.548171000	4.252300000	2.461635000
H	2.557622000	2.786338000	2.512707000
C	1.599470000	4.702632000	-0.253221000
H	2.070062000	5.080203000	-1.170956000
H	1.288665000	5.575087000	0.341541000
H	0.698272000	4.140310000	-0.528246000
H	4.350882000	-5.771340000	-0.061386000
H	4.002211000	-1.847640000	3.249138000
H	5.687501000	-2.268850000	2.924296000
H	6.973875000	2.337502000	2.870457000
H	0.014448000	-0.697071000	0.306071000
N	-2.045152000	4.340034000	3.453459000
N	-1.749697000	3.984048000	2.439011000

$TS_{HH'}$(closed-shell singlet)

Ti	-1.300195000	-0.065569000	-0.497640000
Ti	1.413342000	-0.300738000	-0.027844000
P	-2.337959000	-2.520777000	-0.204256000
P	1.630434000	0.298763000	2.511386000
P	3.486085000	-1.632021000	-1.081554000
P	-2.560478000	1.653133000	-2.090700000
N	3.087019000	1.025469000	0.074974000
N	-3.166997000	0.276291000	0.455514000
N	-0.049171000	1.210966000	0.065061000
N	0.314742000	0.676446000	-1.213435000
C	3.097393000	2.082634000	1.004265000
C	-3.444308000	-2.066036000	1.183193000
C	-4.718868000	1.971129000	1.382475000
C	2.520206000	2.929993000	3.233490000
H	2.024721000	2.792109000	4.194292000
C	-4.435359000	3.498914000	-0.952902000
H	-4.298458000	4.112543000	-1.842906000
C	4.136223000	1.026238000	-0.858626000
C	-3.863373000	1.500334000	0.351309000
C	-3.709425000	-0.670364000	1.354327000
C	3.147065000	-2.403649000	-2.769803000
H	4.124535000	-2.622466000	-3.228469000
C	-5.156473000	-1.243251000	3.244499000
H	-5.816986000	-0.910776000	4.047222000
C	-3.727705000	2.289301000	-0.829191000
C	2.470392000	1.907174000	2.270670000
C	4.530683000	-0.190359000	-1.492350000
C	3.201387000	4.126496000	2.977808000
C	4.322278000	3.523315000	-0.642787000
C	4.845695000	2.215717000	-1.192897000
C	3.759626000	3.312123000	0.743933000
C	6.330642000	0.960208000	-2.675523000
C	-2.958480000	0.142167000	-4.483740000
H	-2.206665000	0.658716000	-5.094102000
H	-3.684225000	-0.319569000	-5.169812000
H	-2.447695000	-0.659556000	-3.934960000
C	-1.229768000	-3.965796000	0.346749000
H	-0.398835000	-3.892391000	-0.372168000
C	-5.441166000	3.157050000	1.211292000
H	-6.099368000	3.490361000	2.015507000
C	-3.503700000	-3.326342000	-1.460394000
H	-3.891240000	-4.243504000	-0.990773000
C	5.935691000	2.161052000	-2.065548000
H	6.467668000	3.086037000	-2.295521000
C	-4.561054000	-0.278603000	2.425234000
C	-1.644756000	3.188654000	-2.699035000
H	-2.402367000	3.830141000	-3.178073000
C	-5.306925000	3.932653000	0.052011000
C	3.817363000	4.301778000	1.731055000
H	4.336078000	5.235708000	1.507286000
C	-0.634766000	-3.730322000	1.748765000
H	-0.134257000	-2.757680000	1.804337000
H	0.105946000	-4.515784000	1.963663000
H	-1.408883000	-3.769467000	2.526527000
C	4.232497000	-0.655343000	2.988161000
H	4.194441000	-0.889149000	1.917566000
H	4.888846000	-1.384452000	3.486491000
H	4.683306000	0.340727000	3.089502000
C	5.607931000	-0.204238000	-2.397677000
H	5.879483000	-1.134206000	-2.897231000
C	-4.756150000	1.198770000	2.681156000
C	4.622286000	-2.849603000	-0.162875000
H	5.180747000	-2.182586000	0.510168000
C	-2.731993000	-3.699661000	-2.742313000
H	-2.324854000	-2.802594000	-3.228025000
H	-3.404436000	-4.195236000	-3.458363000
H	-1.891737000	-4.378610000	-2.544644000
C	-4.046478000	-3.007798000	2.038839000
H	-3.851701000	-4.067947000	1.886021000
C	0.202280000	0.683608000	3.678021000
H	0.671533000	1.079705000	4.592204000
C	2.402649000	-1.379402000	-3.651234000
H	1.445879000	-1.097204000	-3.190441000
H	2.195723000	-1.823549000	-4.637044000
H	2.994124000	-0.467835000	-3.801206000
C	-3.682983000	1.114047000	-3.528681000
H	-4.468423000	0.551260000	-3.001155000
C	-0.573287000	2.813522000	-3.744970000
H	0.153681000	2.117025000	-3.308753000
H	-0.040473000	3.723245000	-4.060381000
H	-1.007093000	2.356812000	-4.644305000
C	-4.362089000	2.255148000	-4.307954000
H	-4.937775000	2.914857000	-3.647255000
H	-5.059750000	1.832130000	-5.046711000
H	-3.628895000	2.861299000	-4.857727000
C	-4.909208000	-2.610884000	3.065002000
C	-1.828638000	-5.385573000	0.253190000
H	-2.661927000	-5.530666000	0.953624000
H	-1.049503000	-6.115454000	0.520482000
H	-2.182327000	-5.639099000	-0.753274000
C	-0.753576000	1.757676000	3.126937000
H	-0.222630000	2.674532000	2.846843000
H	-1.492684000	2.007077000	3.904832000
H	-1.286118000	1.397685000	2.240503000
C	2.339577000	-3.711447000	-2.663227000
H	2.882035000	-4.499146000	-2.124034000
H	2.117786000	-4.090481000	-3.672440000
H	1.388184000	-3.525349000	-2.147146000
C	2.829159000	-0.678292000	3.626131000
H	2.449166000	-1.712873000	3.598810000

C	-0.564873000	-0.601690000	4.046538000
H	-1.071115000	-1.014976000	3.165919000
H	-1.333521000	-0.372050000	4.799408000
H	0.090482000	-1.379127000	4.464536000
C	5.646589000	-3.592986000	-1.040740000
H	5.159161000	-4.267771000	-1.757263000
H	6.301244000	-4.205902000	-0.402458000
H	6.285192000	-2.896381000	-1.597636000
C	-4.698200000	-2.407636000	-1.772225000
H	-5.284672000	-2.191443000	-0.871128000
H	-5.358049000	-2.891160000	-2.508346000
H	-4.361223000	-1.452625000	-2.194313000
C	-1.011431000	3.969997000	-1.529452000
H	-1.769196000	4.321410000	-0.818364000
H	-0.487100000	4.849182000	-1.934611000
H	-0.292841000	3.348976000	-0.982077000
C	2.911673000	-0.219847000	5.094158000
H	3.212414000	0.835224000	5.158943000
H	3.673894000	-0.813955000	5.621509000
H	1.963953000	-0.346963000	5.632653000
C	3.802040000	-3.824107000	0.709319000
H	3.107171000	-3.284945000	1.366902000
H	4.477655000	-4.421702000	1.339765000
H	3.212824000	-4.520318000	0.098077000
H	-0.178078000	-1.053032000	0.630795000
H	7.170040000	0.940468000	-3.369010000
H	5.105688000	4.295010000	-0.641446000
H	3.516710000	3.893991000	-1.306024000
H	3.243391000	4.910909000	3.732079000
H	-5.859250000	4.864587000	-0.058528000
H	-5.696666000	1.381431000	3.221122000
H	-3.944633000	1.562448000	3.339303000
H	-5.378376000	-3.350237000	3.712298000
H	0.812935000	-1.726126000	-0.884694000

H'(closed-shell singlet)

Ti	1.272361000	0.246240000	-0.330875000
Ti	-1.536568000	0.060270000	0.273551000
P	2.413520000	1.904741000	1.485647000
P	-1.746603000	-2.080769000	1.675611000
P	-2.901611000	2.245817000	0.070748000
P	2.477642000	-0.012395000	-2.688958000
N	-3.387623000	-0.687467000	-0.375072000
N	3.117718000	-0.705555000	0.118774000
N	-0.167708000	-0.720683000	-0.942796000
N	-0.373679000	0.698103000	-1.181828000
C	-3.725730000	-2.059151000	-0.262859000
C	3.543870000	0.617919000	2.153701000
C	4.596032000	-2.633993000	-0.346391000
C	-3.460670000	-4.221990000	0.880692000
H	-2.950827000	-4.831498000	1.626279000
C	4.242887000	-2.238200000	-3.101371000
H	4.083548000	-2.106286000	-4.171347000
C	-4.286580000	0.126690000	-1.104081000
C	3.759313000	-1.576249000	-0.790034000
C	3.733349000	-0.568802000	1.381033000
C	-2.334769000	3.784003000	-0.867926000
H	-3.150255000	4.524266000	-0.833429000
C	5.274055000	-1.380859000	3.100889000
H	5.935008000	-2.168830000	3.465893000
C	3.590510000	-1.384215000	-2.193300000
C	-3.089721000	-2.875399000	0.720644000
C	-4.242389000	1.548489000	-0.968187000
C	-4.465847000	-4.794823000	0.094174000
C	-5.232270000	-1.898038000	-2.278056000
C	-5.266753000	-0.419084000	-1.979752000
C	-4.693487000	-2.674848000	-1.102045000
C	-6.154953000	1.803740000	-2.471878000
C	3.007004000	2.693695000	-3.438106000
H	2.269832000	2.757211000	-4.248886000
H	3.771801000	3.462750000	-3.623221000
H	2.491858000	2.938350000	-2.500194000
C	1.344620000	2.513709000	2.940585000
H	0.449340000	2.893065000	2.425324000
C	5.262382000	-3.440578000	-1.275167000
H	5.906484000	-4.241515000	-0.908302000
C	3.584988000	3.350010000	1.124737000
H	3.977814000	3.683453000	2.097656000
C	-6.192044000	0.412387000	-2.620038000
H	-6.938056000	-0.046034000	-3.271664000
C	4.586545000	-1.582946000	1.900800000
C	1.517715000	-0.685943000	-4.167895000
H	2.251648000	-0.853397000	-4.972755000
C	5.090310000	-3.258318000	-2.654159000
C	-5.065809000	-4.008622000	-0.896278000
H	-5.823565000	-4.442970000	-1.550902000
C	0.893277000	1.339140000	3.833459000
H	0.423212000	0.549698000	3.237365000
H	0.151609000	1.707401000	4.558389000
H	1.737626000	0.915186000	4.392394000
C	-3.794441000	-1.148791000	3.366237000
H	-3.709889000	-0.217147000	2.794362000
H	-4.133353000	-0.907383000	4.385125000
H	-4.555972000	-1.783283000	2.892524000
C	-5.160437000	2.359049000	-1.660982000
H	-5.092728000	3.442440000	-1.565276000
C	4.672413000	-2.888395000	1.141843000
C	-3.816551000	2.835545000	1.625475000
H	-4.297957000	1.897285000	1.942810000
C	2.828566000	4.516775000	0.458937000
H	2.441450000	4.219531000	-0.525003000
H	3.508111000	5.369142000	0.309666000
H	1.978333000	4.866123000	1.059270000
C	4.240377000	0.779908000	3.367140000
H	4.108952000	1.697508000	3.938632000
C	-0.422672000	-3.407034000	1.842887000
H	-0.884386000	-4.270724000	2.347025000
C	-2.020925000	3.444145000	-2.340563000
H	-1.257090000	2.658873000	-2.396884000
H	-1.641953000	4.346293000	-2.845816000
H	-2.909567000	3.096875000	-2.880209000
C	3.667762000	1.300327000	-3.377448000
H	4.444248000	1.325029000	-2.597038000
C	0.469540000	0.340600000	-4.648400000
H	-0.228024000	0.583598000	-3.836976000
H	-0.103293000	-0.088205000	-5.484324000
H	0.928649000	1.271668000	-5.005360000
C	4.347772000	0.945660000	-4.712186000
H	4.874949000	-0.014841000	-4.658597000
H	5.088348000	1.719166000	-4.966189000
H	3.621849000	0.902674000	-5.536017000
C	5.115434000	-0.201628000	3.842350000
C	1.924200000	3.653558000	3.804362000
H	2.814158000	3.335418000	4.364034000
H	1.167180000	3.954589000	4.544014000
H	2.187823000	4.545538000	3.223007000
C	0.084461000	-3.857713000	0.459263000
H	-0.725888000	-4.279293000	-0.148574000
H	0.857550000	-4.631215000	0.586260000
H	0.520441000	-3.017017000	-0.093341000
C	-1.084776000	4.388245000	-0.194118000
H	-1.275904000	4.719161000	0.834009000
H	-0.741279000	5.261668000	-0.769119000
H	-0.272066000	3.650118000	-0.174984000
C	-2.436867000	-1.875968000	3.428877000
H	-1.711368000	-1.205368000	3.914704000
C	0.732624000	-2.883881000	2.720215000
H	1.204751000	-2.007081000	2.258701000

H	1.498755000	-3.665966000	2.830620000
H	0.398543000	-2.599272000	3.727524000
C	-4.914537000	3.888285000	1.388382000
H	-4.493004000	4.840960000	1.035816000
H	-5.435785000	4.093052000	2.335838000
H	-5.661629000	3.545956000	0.662717000
C	4.773764000	2.896470000	0.257767000
H	5.353014000	2.105723000	0.749126000
H	5.441877000	3.750407000	0.069706000
H	4.431818000	2.516446000	-0.713480000
C	0.838347000	-2.030268000	-3.833430000
H	1.568134000	-2.796294000	-3.543442000
H	0.300564000	-2.388188000	-4.724639000
H	0.120977000	-1.907026000	-3.013034000
C	-2.561879000	-3.176123000	4.245433000
H	-3.261805000	-3.876300000	3.768695000
H	-2.960745000	-2.942039000	5.244239000
H	-1.600207000	-3.686418000	4.385347000
C	-2.862097000	3.269197000	2.755746000
H	-2.064327000	2.529501000	2.896052000
H	-3.426680000	3.356093000	3.696460000
H	-2.414169000	4.251983000	2.553401000
H	0.176112000	0.251026000	1.174068000
H	-6.871455000	2.439968000	-2.989132000
H	-6.229361000	-2.262494000	-2.566649000
H	-4.576780000	-2.073266000	-3.153581000
H	-4.757111000	-5.834865000	0.233069000
H	5.597961000	-3.907247000	-3.366137000
H	5.588493000	-3.437047000	1.403531000
H	3.824464000	-3.534814000	1.439953000
H	5.656729000	-0.055601000	4.775807000
H	-1.765647000	0.594659000	1.931092000

$TS_{H'I}$(closed-shell singlet)

Ti	1.639837000	0.242783000	-0.452153000
Ti	-1.704326000	0.415199000	0.499609000
P	2.972525000	2.295067000	0.545692000
P	-2.207420000	-1.021724000	2.505269000
P	-3.031334000	2.233678000	-0.660150000
P	2.194237000	-1.361909000	-2.325746000
N	-3.286076000	-0.775976000	-0.236945000
N	3.489853000	-0.636604000	0.240634000
N	0.088753000	-0.491396000	0.124007000
N	-0.150387000	0.614147000	-0.794291000
C	-3.743664000	-1.943634000	0.404238000
C	4.311301000	1.385869000	1.388754000
C	4.751112000	-2.756887000	0.551504000
C	-3.885695000	-3.350456000	2.408996000
H	-3.592596000	-3.548238000	3.440376000
C	3.755778000	-3.710806000	-1.890553000
H	3.344512000	-4.092292000	-2.824972000
C	-4.097515000	-0.295128000	-1.278300000
C	3.867824000	-1.929980000	-0.193377000
C	4.343455000	-0.029909000	1.187747000
C	-2.348138000	3.379949000	-2.005389000
H	-3.189008000	3.957737000	-2.421499000
C	6.211709000	-0.129785000	2.769858000
H	6.929660000	-0.735304000	3.325624000
C	3.372044000	-2.437482000	-1.433339000
C	-3.380800000	-2.210672000	1.755888000
C	-4.132548000	1.098807000	-1.598312000
C	-4.752290000	-4.234215000	1.756682000
C	-4.816071000	-2.654582000	-1.742327000
C	-4.935277000	-1.174539000	-2.025159000
C	-4.580399000	-2.877994000	-0.266643000
C	-5.805371000	0.687239000	-3.340200000
C	2.564146000	0.610160000	-4.368386000
H	1.671673000	0.366458000	-4.958084000
H	3.279340000	1.111154000	-5.037460000
H	2.260826000	1.327787000	-3.593359000
C	2.079369000	3.373396000	1.816540000
H	1.151120000	3.646889000	1.291184000
C	5.145878000	-4.003656000	0.052854000
H	5.832258000	-4.609078000	0.647166000
C	3.840753000	3.489548000	-0.626503000
H	4.438477000	4.165872000	0.004377000
C	-5.783500000	-0.677593000	-3.016755000
H	-6.419255000	-1.377407000	-3.562196000
C	5.280650000	-0.779887000	1.954111000
C	0.895376000	-2.511688000	-3.054666000
H	1.427581000	-3.185252000	-3.745522000
C	4.655434000	-4.496880000	-1.162789000
C	-5.086579000	-3.987257000	0.416198000
H	-5.734837000	-4.682892000	-0.119904000
C	1.684810000	2.514645000	3.034958000
H	1.038399000	1.680308000	2.736780000
H	1.113797000	3.133867000	3.741967000
H	2.572635000	2.127890000	3.553210000
C	-4.562018000	0.072185000	3.650829000
H	-4.641871000	0.618973000	2.703825000
H	-5.006136000	0.684143000	4.450835000
H	-5.141708000	-0.857192000	3.566364000
C	-4.967275000	1.557323000	-2.637386000
H	-4.964336000	2.615977000	-2.895624000
C	5.182097000	-2.286805000	1.920502000
C	-4.175923000	3.311896000	0.397972000
H	-4.843807000	2.546480000	0.820124000
C	2.814584000	4.318350000	-1.423976000
H	2.188975000	3.670981000	-2.054522000
H	3.337036000	5.027440000	-2.082772000
H	2.146952000	4.895228000	-0.770886000
C	5.255955000	2.009959000	2.225933000
H	5.238619000	3.092938000	2.336427000
C	-0.882608000	-2.127772000	3.282710000
H	-1.353282000	-2.677298000	4.113094000
C	-1.697872000	2.564366000	-3.140862000
H	-0.898649000	1.923372000	-2.747864000
H	-1.266133000	3.251510000	-3.886045000
H	-2.429204000	1.924402000	-3.649304000
C	3.213282000	-0.652139000	-3.761665000
H	4.136004000	-0.344984000	-3.243499000
C	-0.170827000	-1.722512000	-3.843349000
H	-0.655027000	-0.975417000	-3.202348000
H	-0.942807000	-2.418795000	-4.202511000
H	0.249158000	-1.213097000	-4.719969000
C	3.591950000	-1.673797000	-4.849376000
H	4.110309000	-2.542887000	-4.425607000
H	4.267158000	-1.204338000	-5.580332000
H	2.706225000	-2.025359000	-5.396712000
C	6.226618000	1.265687000	2.902022000
C	2.797944000	4.666704000	2.249426000
H	3.695995000	4.453030000	2.843060000
H	2.117766000	5.251100000	2.886331000
H	3.084387000	5.303685000	1.402376000
C	-0.335319000	-3.150421000	2.268122000
H	-1.121996000	-3.824428000	1.906991000
H	0.445751000	-3.760518000	2.748645000
H	0.109469000	-2.641474000	1.404355000
C	-1.329518000	4.365210000	-1.396552000
H	-1.789439000	5.042410000	-0.665782000
H	-0.884613000	4.983323000	-2.191832000
H	-0.521445000	3.816287000	-0.893885000
C	-3.088627000	-0.227627000	3.991532000
H	-2.558268000	0.730668000	4.098821000
C	0.260424000	-1.253696000	3.837224000
H	0.752791000	-0.718281000	3.015599000
H	1.009918000	-1.886404000	4.337420000
H	-0.090788000	-0.507178000	4.563007000

C	-5.024177000	4.343540000	-0.366140000
H	-4.401559000	5.128582000	-0.819179000
H	-5.716474000	4.838451000	0.331843000
H	-5.626850000	3.877257000	-1.155830000
C	4.801785000	2.727268000	-1.559248000
H	5.544907000	2.154922000	-0.990746000
H	5.333380000	3.440059000	-2.206814000
H	4.255118000	2.028647000	-2.207538000
C	0.234713000	-3.354144000	-1.944102000
H	0.969714000	-3.951271000	-1.390512000
H	-0.492657000	-4.041130000	-2.401730000
H	-0.293842000	-2.708981000	-1.232565000
C	-3.004723000	-1.006625000	5.319193000
H	-3.496681000	-1.986801000	5.242224000
H	-3.529848000	-0.440022000	6.103357000
H	-1.973939000	-1.163826000	5.660127000
C	-3.408644000	3.955048000	1.572096000
H	-2.781588000	3.207948000	2.075337000
H	-4.125675000	4.367993000	2.298177000
H	-2.768689000	4.782571000	1.234996000
H	-1.047797000	1.389319000	1.815692000
H	-6.457679000	1.061534000	-4.127944000
H	-5.704337000	-3.198871000	-2.093691000
H	-3.953597000	-3.061052000	-2.307632000
H	-5.144067000	-5.109660000	2.272807000
H	4.957343000	-5.477120000	-1.527822000
H	6.134064000	-2.751273000	2.215575000
H	4.432572000	-2.613546000	2.667468000
H	6.962644000	1.757394000	3.535734000
H	-3.044102000	1.032101000	1.446150000

I(closed-shell singlet)

Ti	1.699792000	0.295973000	-0.458770000
Ti	-1.726405000	0.549272000	0.578922000
P	3.133638000	2.302066000	0.384727000
P	-2.313370000	-0.820658000	2.609748000
P	-3.058675000	2.238488000	-0.735760000
P	2.042589000	-1.528154000	-2.191944000
N	-3.175088000	-0.764174000	-0.225124000
N	3.532521000	-0.658468000	0.216895000
N	0.190409000	-0.172811000	0.432378000
N	-0.083992000	0.793530000	-0.608438000
C	-3.622198000	-1.924166000	0.437743000
C	4.486039000	1.394413000	1.202249000
C	4.713269000	-2.811997000	0.627205000
C	-3.832174000	-3.253040000	2.489462000
H	-3.603596000	-3.391483000	3.546466000
C	3.532193000	-3.901715000	-1.669609000
H	3.047473000	-4.333278000	-2.545201000
C	-3.943893000	-0.363227000	-1.331899000
C	3.825607000	-1.999387000	-0.129536000
C	4.453070000	-0.031657000	1.085782000
C	-2.332100000	3.376521000	-2.065588000
H	-3.166138000	3.902965000	-2.556848000
C	6.400805000	-0.107217000	2.573359000
H	7.123231000	-0.706909000	3.129756000
C	3.232343000	-2.580793000	-1.292141000
C	-3.345731000	-2.112739000	1.823006000
C	-4.026720000	1.014456000	-1.708486000
C	-4.601863000	-4.210081000	1.819458000
C	-4.522263000	-2.772168000	-1.739502000
C	-4.688399000	-1.311528000	-2.092579000
C	-4.365940000	-2.926501000	-0.244423000
C	-5.554107000	0.452167000	-3.539526000
C	2.363362000	0.279377000	-4.388645000
H	1.410067000	0.046165000	-4.878733000
H	3.042660000	0.683556000	-5.153758000
H	2.168896000	1.073912000	-3.654207000
C	2.293223000	3.431603000	1.641258000
H	1.425242000	3.810999000	1.079596000
C	5.021378000	-4.111277000	0.207667000
H	5.713603000	-4.701855000	0.810180000
C	3.977325000	3.450208000	-0.848983000
H	4.654443000	4.092820000	-0.264657000
C	-5.490014000	-0.896216000	-3.158048000
H	-6.054434000	-1.647323000	-3.713696000
C	5.400959000	-0.768173000	1.853223000
C	0.660083000	-2.675202000	-2.745305000
H	1.125940000	-3.447756000	-3.377764000
C	4.439390000	-4.672730000	-0.935559000
C	-4.858881000	-4.033910000	0.451147000
H	-5.434992000	-4.783138000	-0.095049000
C	1.756934000	2.586911000	2.814248000
H	1.025348000	1.846758000	2.468275000
H	1.245524000	3.246025000	3.530700000
H	2.575769000	2.077427000	3.340982000
C	-4.817104000	0.180442000	3.497659000
H	-4.841509000	0.687035000	2.525587000
H	-5.362450000	0.794771000	4.230314000
H	-5.336864000	-0.782641000	3.401378000
C	-4.810045000	1.390211000	-2.818358000
H	-4.841374000	2.437476000	-3.118096000
C	5.244516000	-2.267824000	1.931370000
C	-4.334815000	3.290053000	0.190928000
H	-4.999929000	2.505796000	0.581724000
C	2.947438000	4.335950000	-1.577515000
H	2.228947000	3.725940000	-2.143278000
H	3.461552000	4.998081000	-2.289605000
H	2.377861000	4.967237000	-0.883261000
C	5.502444000	2.030976000	1.940379000
H	5.535126000	3.118700000	1.975696000
C	-0.994026000	-1.801933000	3.545604000
H	-1.498824000	-2.356897000	4.352026000
C	-1.567773000	2.562037000	-3.128364000
H	-0.767479000	1.973978000	-2.661749000
H	-1.118601000	3.248056000	-3.864257000
H	-2.230763000	1.871819000	-3.664346000
C	2.995896000	-0.967988000	-3.735094000
H	3.963376000	-0.669750000	-3.299880000
C	-0.401411000	-1.923342000	-3.575038000
H	-0.820430000	-1.082952000	-3.008006000
H	-1.223413000	-2.611929000	-3.819288000
H	0.001612000	-1.541625000	-4.521814000
C	3.256434000	-2.081378000	-4.766007000
H	3.766128000	-2.940267000	-4.312007000
H	3.898981000	-1.698091000	-5.572712000
H	2.321584000	-2.430938000	-5.225955000
C	6.481211000	1.291599000	2.609665000
C	3.118336000	4.632648000	2.143198000
H	3.942521000	4.308306000	2.790911000
H	2.466179000	5.283610000	2.743734000
H	3.532426000	5.241499000	1.328185000
C	-0.288231000	-2.813718000	2.622188000
H	-0.989676000	-3.557260000	2.223488000
H	0.490519000	-3.346702000	3.190102000
H	0.191952000	-2.301073000	1.779628000
C	-1.403278000	4.423191000	-1.415974000
H	-1.943354000	5.095446000	-0.737358000
H	-0.933145000	5.042109000	-2.196052000
H	-0.608647000	3.925689000	-0.843130000
C	-3.366333000	-0.023319000	3.977622000
H	-2.899256000	0.966431000	4.092832000
C	0.030137000	-0.827723000	4.162140000
H	0.554977000	-0.285440000	3.366144000
H	0.773577000	-1.386495000	4.751289000
H	-0.437235000	-0.085393000	4.823888000
C	-5.163934000	4.257248000	-0.672598000
H	-4.543181000	5.060512000	-1.094911000

H	-5.934947000	4.734758000	-0.048988000
H	-5.675946000	3.742329000	-1.495482000
C	4.828139000	2.633955000	-1.841965000
H	5.562517000	2.006431000	-1.321915000
H	5.369116000	3.314048000	-2.516253000
H	4.197801000	1.981461000	-2.462717000
C	0.016444000	-3.354470000	-1.518820000
H	0.752406000	-3.915083000	-0.929560000
H	-0.757499000	-4.057115000	-1.861395000
H	-0.456800000	-2.611741000	-0.865972000
C	-3.360871000	-0.749800000	5.337353000
H	-3.791215000	-1.758162000	5.255906000
H	-3.983823000	-0.186806000	6.049094000
H	-2.358151000	-0.836635000	5.773541000
C	-3.699473000	4.005048000	1.401550000
H	-3.076790000	3.307792000	1.976086000
H	-4.494028000	4.399425000	2.053535000
H	-3.077018000	4.855536000	1.090186000
H	-1.287677000	1.672774000	1.859345000
H	-6.167767000	0.762271000	-4.384170000
H	-5.364118000	-3.369744000	-2.117699000
H	-3.612019000	-3.162353000	-2.237101000
H	-4.980852000	-5.085001000	2.345888000
H	4.675493000	-5.691552000	-1.238017000
H	6.195123000	-2.750018000	2.201758000
H	4.531534000	-2.512651000	2.742747000
H	7.272890000	1.790661000	3.165795000
H	-3.185037000	1.104616000	1.367869000

TS_{IJ}(closed-shell singlet)

Ti	1.641264000	0.318828000	-0.516721000
Ti	-1.702041000	0.678587000	0.699831000
P	2.966510000	2.379696000	0.211612000
P	-2.144989000	-0.852749000	2.650870000
P	-3.220214000	2.142265000	-0.722718000
P	2.021448000	-1.631105000	-2.102808000
N	-3.184641000	-0.709591000	-0.084463000
N	3.545199000	-0.537926000	0.170342000
N	0.183571000	0.021884000	0.575390000
N	-0.165337000	0.837053000	-0.564184000
C	-3.376395000	-2.000467000	0.482185000
C	4.426516000	1.615184000	0.990401000
C	4.855747000	-2.600582000	0.670087000
C	-3.188171000	-3.514306000	2.421665000
H	-2.857420000	-3.684142000	3.446339000
C	3.635945000	-3.903153000	-1.491009000
H	3.139097000	-4.414935000	-2.315371000
C	-3.959509000	-0.443905000	-1.244486000
C	3.896216000	-1.883295000	-0.097190000
C	4.468848000	0.185558000	0.958174000
C	-2.544876000	3.329075000	-2.022864000
H	-3.412873000	3.768289000	-2.540029000
C	6.478344000	0.310182000	2.360454000
H	7.255201000	-0.214239000	2.919935000
C	3.288305000	-2.574716000	-1.190540000
C	-2.978460000	-2.256947000	1.830456000
C	-4.151179000	0.901503000	-1.686098000
C	-3.809392000	-4.551784000	1.717678000
C	-4.270996000	-2.908970000	-1.698521000
C	-4.582322000	-1.467792000	-2.014542000
C	-3.969844000	-3.080010000	-0.230920000
C	-5.595153000	0.176776000	-3.518093000
C	2.216175000	0.063458000	-4.402868000
H	1.248575000	-0.219799000	-4.835658000
H	2.850736000	0.439529000	-5.219267000
H	2.033199000	0.895625000	-3.707658000
C	2.097254000	3.450416000	1.506519000
H	1.129992000	3.673096000	1.030038000
C	5.207358000	-3.911839000	0.328290000
H	5.952332000	-4.425248000	0.938895000
C	3.668160000	3.591709000	-1.054306000
H	4.293804000	4.311022000	-0.502704000
C	-5.398615000	-1.146319000	-3.105781000
H	-5.865473000	-1.962811000	-3.660180000
C	5.489083000	-0.447995000	1.725534000
C	0.678303000	-2.868396000	-2.542393000
H	1.157894000	-3.676003000	-3.118049000
C	4.606650000	-4.580423000	-0.745324000
C	-4.193276000	-4.314001000	0.393549000
H	-4.657950000	-5.111670000	-0.189386000
C	1.819447000	2.604305000	2.764823000
H	1.263228000	1.694475000	2.510304000
H	1.216791000	3.189856000	3.474545000
H	2.758097000	2.320304000	3.260257000
C	-4.677523000	0.260718000	3.117188000
H	-4.415880000	0.996711000	2.345046000
H	-5.397217000	0.730375000	3.804551000
H	-5.174954000	-0.583370000	2.620862000
C	-4.945431000	1.191982000	-2.808360000
H	-5.047642000	2.226208000	-3.137821000
C	5.419829000	-1.944854000	1.907137000
C	-4.579658000	3.092761000	0.213836000
H	-5.218456000	2.271922000	0.575892000
C	2.535584000	4.352034000	-1.771521000
H	1.868429000	3.656267000	-2.300182000
H	2.958202000	5.046111000	-2.513206000
H	1.920834000	4.937217000	-1.075034000
C	5.432228000	2.351752000	1.643917000
H	5.399920000	3.440299000	1.615233000
C	-0.825764000	-1.631728000	3.744415000
H	-1.344512000	-2.352525000	4.396258000
C	-1.692999000	2.565112000	-3.057227000
H	-0.845811000	2.070095000	-2.567446000
H	-1.306813000	3.274235000	-3.806076000
H	-2.281868000	1.801150000	-3.579586000
C	2.908799000	-1.127463000	-3.706432000
H	3.879730000	-0.776595000	-3.321088000
C	-0.421759000	-2.223309000	-3.409813000
H	-0.872050000	-1.362746000	-2.898801000
H	-1.215040000	-2.961660000	-3.597875000
H	-0.042835000	-1.891856000	-4.385071000
C	3.173722000	-2.286693000	-4.683982000
H	3.724077000	-3.102877000	-4.199504000
H	3.779019000	-1.930187000	-5.531000000
H	2.237255000	-2.690549000	-5.093636000
C	6.480180000	1.710796000	2.311298000
C	2.790308000	4.776782000	1.873649000
H	3.736028000	4.600922000	2.402408000
H	2.136477000	5.345133000	2.551976000
H	2.991870000	5.411767000	1.001005000
C	0.219273000	-2.398389000	2.910267000
H	-0.249245000	-3.185295000	2.305752000
H	0.946655000	-2.873921000	3.586310000
H	0.758035000	-1.722970000	2.236084000
C	-1.728650000	4.462294000	-1.370916000
H	-2.344760000	5.097726000	-0.721676000
H	-1.295358000	5.104270000	-2.153258000
H	-0.912489000	4.044589000	-0.767584000
C	-3.431676000	-0.213006000	3.890866000
H	-2.947681000	0.669334000	4.338537000
C	-0.159017000	-0.563953000	4.634545000
H	0.333173000	0.200313000	4.021376000
H	0.602968000	-1.037571000	5.271723000
H	-0.880898000	-0.061290000	5.292868000
C	-5.450105000	4.014061000	-0.661141000
H	-4.870267000	4.856622000	-1.063695000
H	-6.265246000	4.436159000	-0.053856000
H	-5.906022000	3.471394000	-1.498241000

C	4.566941000	2.843354000	-2.058596000
H	5.379454000	2.309223000	-1.550643000
H	5.010976000	3.556501000	-2.768926000
H	3.988241000	2.111448000	-2.640740000
C	0.083017000	-3.459880000	-1.247422000
H	0.849844000	-3.953361000	-0.637496000
H	-0.684808000	-4.204460000	-1.504221000
H	-0.388511000	-2.676574000	-0.641512000
C	-3.830205000	-1.194518000	5.007131000
H	-4.289211000	-2.100365000	4.588310000
H	-4.571279000	-0.720766000	5.669303000
H	-2.975682000	-1.493140000	5.628812000
C	-4.032067000	3.847646000	1.444112000
H	-3.444558000	3.192425000	2.099344000
H	-4.870782000	4.257605000	2.027526000
H	-3.387614000	4.687254000	1.152715000
H	-1.386208000	2.343078000	1.205785000
H	-6.219232000	0.407231000	-4.380306000
H	-5.096808000	-3.566584000	-2.009515000
H	-3.390229000	-3.227906000	-2.290183000
H	-3.976685000	-5.522169000	2.182897000
H	4.878470000	-5.606917000	-0.986007000
H	6.407761000	-2.358760000	2.157202000
H	4.762992000	-2.172353000	2.769847000
H	7.264167000	2.285667000	2.801573000
H	-1.354062000	1.726879000	2.103643000

TS_{IJ}(triplet)

Ti	-1.724033000	0.180811000	0.153809000
Ti	1.847258000	0.513761000	-0.862052000
P	-3.173318000	2.252446000	-0.354656000
P	2.531339000	-1.408631000	-2.358466000
P	3.100065000	2.391031000	0.315446000
P	-2.184175000	-1.347358000	2.134101000
N	3.363318000	-0.534031000	0.318322000
N	-3.556602000	-0.687298000	-0.378121000
N	0.095216000	-0.306401000	-0.527485000
N	0.216063000	0.803019000	0.193419000
C	3.713480000	-1.887702000	0.068181000
C	-4.564899000	1.393945000	-1.191206000
C	-4.834269000	-2.792388000	-0.641554000
C	3.847973000	-3.796942000	-1.493754000
H	3.621333000	-4.220063000	-2.472460000
C	-3.679135000	-3.775857000	1.723729000
H	-3.223757000	-4.166805000	2.633573000
C	3.991153000	0.052899000	1.447532000
C	-3.908537000	-1.982745000	0.066217000
C	-4.531982000	-0.032099000	-1.157949000
C	2.263245000	3.792140000	1.254572000
H	3.061964000	4.374455000	1.741179000
C	-6.545169000	-0.069863000	-2.540563000
H	-7.300780000	-0.645045000	-3.078421000
C	-3.341578000	-2.486654000	1.274206000
C	3.457770000	-2.476600000	-1.209623000
C	4.025789000	1.474224000	1.593777000
C	4.509988000	-4.577006000	-0.540329000
C	4.452174000	-2.212584000	2.459599000
C	4.615571000	-0.713723000	2.472965000
C	4.331701000	-2.720047000	1.044909000
C	5.339150000	1.307325000	3.647266000
C	-2.593757000	0.596756000	4.190767000
H	-1.705020000	0.368873000	4.793266000
H	-3.323035000	1.090269000	4.850528000
H	-2.297259000	1.310488000	3.409496000
C	-2.293136000	3.246902000	-1.712554000
H	-1.389772000	3.619947000	-1.206302000
C	-5.177820000	-4.056925000	-0.149409000
H	-5.894890000	-4.661406000	-0.707473000
C	-4.001147000	3.562794000	0.727112000
H	-4.600106000	4.204216000	0.061807000
C	5.291897000	-0.086215000	3.525828000
H	5.765945000	-0.713931000	4.282808000
C	-5.519170000	-0.754670000	-1.880600000
C	-0.869307000	-2.477883000	2.876356000
H	-1.383031000	-3.182332000	3.549777000
C	-4.600230000	-4.564362000	1.022713000
C	4.737391000	-4.021130000	0.724180000
H	5.218434000	-4.618387000	1.501193000
C	-1.842125000	2.280229000	-2.827657000
H	-1.181169000	1.488419000	-2.448609000
H	-1.271075000	2.832281000	-3.588453000
H	-2.708595000	1.814600000	-3.317347000
C	4.924401000	-0.125986000	-3.050740000
H	4.552640000	0.745109000	-2.494764000
H	5.619579000	0.238527000	-3.821849000
H	5.487069000	-0.758050000	-2.350503000
C	4.681386000	2.076097000	2.681671000
H	4.667816000	3.161667000	2.780183000
C	-5.371003000	-2.259303000	-1.952420000
C	4.470132000	3.185966000	-0.739470000
H	5.151046000	2.333660000	-0.893617000
C	-2.937186000	4.425572000	1.432751000
H	-2.287449000	3.804519000	2.065699000
H	-3.424242000	5.173108000	2.076444000
H	-2.298261000	4.962481000	0.718680000
C	-5.607174000	2.052636000	-1.871641000
H	-5.652260000	3.140923000	-1.861051000
C	1.317669000	-2.533912000	-3.252112000
H	1.915332000	-3.303289000	-3.766561000
C	1.336759000	3.220399000	2.347902000
H	0.538555000	2.615023000	1.902451000
H	0.880274000	4.050846000	2.908464000
H	1.889890000	2.591832000	3.056800000
C	-3.216826000	-0.676374000	3.581760000
H	-4.143689000	-0.383557000	3.063444000
C	0.165900000	-1.677141000	3.693433000
H	0.645049000	-0.906122000	3.075575000
H	0.951757000	-2.357503000	4.054121000
H	-0.278902000	-1.191571000	4.570934000
C	-3.572313000	-1.712940000	4.662449000
H	-4.064552000	-2.594162000	4.232050000
H	-4.263156000	-1.266768000	5.393799000
H	-2.679918000	-2.043749000	5.212437000
C	-6.607923000	1.331150000	-2.533120000
C	-3.057964000	4.444673000	-2.305401000
H	-3.939883000	4.113983000	-2.869109000
H	-2.401418000	4.981702000	-3.006644000
H	-3.381784000	5.163297000	-1.540749000
C	0.370867000	-3.238809000	-2.261288000
H	0.927090000	-3.836926000	-1.528709000
H	-0.300655000	-3.912615000	-2.815006000
H	-0.239857000	-2.509275000	-1.717760000
C	1.485306000	4.723810000	0.304492000
H	2.149514000	5.263391000	-0.382493000
H	0.933470000	5.472838000	0.892680000
H	0.767123000	4.150505000	-0.295125000
C	3.772167000	-0.915877000	-3.702648000
H	3.203300000	-0.227568000	-4.347072000
C	0.526983000	-1.735484000	-4.309018000
H	-0.043001000	-0.926483000	-3.835150000
H	-0.178219000	-2.404300000	-4.824938000
H	1.182651000	-1.289230000	-5.069367000
C	5.266577000	4.300745000	-0.036048000
H	4.640430000	5.182831000	0.159064000
H	6.097835000	4.623851000	-0.680989000
H	5.695185000	3.957958000	0.913681000
C	-4.950291000	2.894613000	1.739472000
H	-5.725335000	2.305289000	1.233529000

H	-5.445036000	3.663328000	2.351896000
H	-4.398148000	2.226889000	2.414359000
C	-0.171189000	-3.275722000	1.755787000
H	-0.882257000	-3.886056000	1.185232000
H	0.581566000	-3.946231000	2.196816000
H	0.340625000	-2.601240000	1.058068000
C	4.322742000	-2.070600000	-4.558088000
H	4.874417000	-2.790971000	-3.938988000
H	5.021637000	-1.672732000	-5.309779000
H	3.531014000	-2.608314000	-5.096281000
C	3.963538000	3.646172000	-2.123644000
H	3.381327000	2.865426000	-2.629089000
H	4.821588000	3.912013000	-2.759764000
H	3.321057000	4.532710000	-2.045215000
H	1.305874000	0.902646000	-2.486997000
H	5.854237000	1.779250000	4.482599000
H	5.284330000	-2.704300000	2.985351000
H	3.535264000	-2.482228000	3.020584000
H	4.818929000	-5.596307000	-0.767027000
H	-4.862846000	-5.557845000	1.383154000
H	-6.324807000	-2.739557000	-2.213809000
H	-4.660710000	-2.511895000	-2.763932000
H	-7.418543000	1.851022000	-3.041613000
H	1.367221000	2.017696000	-1.619412000

J(closed-shell singlet)

Ti	1.653083000	0.332102000	-0.496903000
Ti	-1.701713000	0.647275000	0.681112000
P	3.008995000	2.354685000	0.247648000
P	-2.157851000	-0.869993000	2.646370000
P	-3.219000000	2.170011000	-0.700364000
P	1.994473000	-1.597693000	-2.114365000
N	-3.195495000	-0.701206000	-0.094116000
N	3.556798000	-0.563473000	0.150808000
N	0.183071000	0.039733000	0.602868000
N	-0.163801000	0.878942000	-0.527722000
C	-3.401734000	-1.993907000	0.464563000
C	4.479963000	1.566743000	0.982470000
C	4.853492000	-2.647642000	0.599265000
C	-3.220333000	-3.522424000	2.390668000
H	-2.890966000	-3.703675000	3.413751000
C	3.591181000	-3.901676000	-1.566203000
H	3.078738000	-4.394029000	-2.392929000
C	-3.974177000	-0.414386000	-1.246685000
C	3.891237000	-1.907875000	-0.143080000
C	4.503558000	0.137347000	0.931982000
C	-2.536976000	3.360880000	-1.994168000
H	-3.400810000	3.811302000	-2.508511000
C	6.536987000	0.218983000	2.303191000
H	7.315525000	-0.322327000	2.844018000
C	3.262128000	-2.574934000	-1.239244000
C	-3.005766000	-2.260354000	1.810955000
C	-4.156548000	0.937874000	-1.671332000
C	-3.845926000	-4.551145000	1.677128000
C	-4.311498000	-2.872206000	-1.721365000
C	-4.608922000	-1.424835000	-2.024163000
C	-4.005324000	-3.061023000	-0.256613000
C	-5.610076000	0.244210000	-3.508069000
C	2.184262000	0.140752000	-4.380934000
H	1.205816000	-0.120134000	-4.803360000
H	2.811272000	0.523670000	-5.200086000
H	2.024746000	0.961873000	-3.666975000
C	2.173250000	3.396788000	1.590144000
H	1.203196000	3.650241000	1.134328000
C	5.185396000	-3.957364000	0.232407000
H	5.932489000	-4.488641000	0.824964000
C	3.700263000	3.609963000	-0.984923000
H	4.340843000	4.305217000	-0.419734000
C	-5.424720000	-1.084924000	-3.110196000
H	-5.900584000	-1.891150000	-3.671853000
C	5.528234000	-0.518548000	1.674082000
C	0.633789000	-2.812261000	-2.562900000
H	1.097602000	-3.614267000	-3.158960000
C	4.563309000	-4.602035000	-0.843613000
C	-4.232933000	-4.300292000	0.356585000
H	-4.702692000	-5.090659000	-0.232118000
C	1.903751000	2.513934000	2.824727000
H	1.343954000	1.612497000	2.547447000
H	1.314182000	3.079535000	3.561796000
H	2.846810000	2.209782000	3.299239000
C	-4.694130000	0.231624000	3.138323000
H	-4.437881000	0.969308000	2.365482000
H	-5.408758000	0.699597000	3.832059000
H	-5.195857000	-0.610075000	2.642332000
C	-4.951132000	1.246619000	-2.788754000
H	-5.046982000	2.285089000	-3.106480000
C	5.442559000	-2.016604000	1.837379000
C	-4.576148000	3.121572000	0.240298000
H	-5.227776000	2.304009000	0.586341000
C	2.561097000	4.402226000	-1.655133000
H	1.878054000	3.728435000	-2.192139000
H	2.974429000	5.116957000	-2.382408000
H	1.964914000	4.969332000	-0.927981000
C	5.505883000	2.282287000	1.627970000
H	5.488399000	3.371529000	1.611384000
C	-0.843783000	-1.677302000	3.726210000
H	-1.367074000	-2.403257000	4.368471000
C	-1.689244000	2.597111000	-3.032052000
H	-0.848859000	2.089461000	-2.543388000
H	-1.293314000	3.308566000	-3.773540000
H	-2.284375000	1.843916000	-3.562821000
C	2.869959000	-1.073205000	-3.718340000
H	3.849948000	-0.742810000	-3.337981000
C	-0.468772000	-2.138863000	-3.405143000
H	-0.903052000	-1.283318000	-2.872323000
H	-1.272632000	-2.864393000	-3.598451000
H	-0.097109000	-1.792671000	-4.378145000
C	3.108034000	-2.215188000	-4.722613000
H	3.653152000	-3.048172000	-4.261302000
H	3.708051000	-1.849450000	-5.569533000
H	2.161640000	-2.598664000	-5.129125000
C	6.555978000	1.619845000	2.271122000
C	2.888872000	4.700934000	1.991690000
H	3.841480000	4.493773000	2.496044000
H	2.255310000	5.253461000	2.701867000
H	3.083296000	5.363689000	1.138398000
C	0.193150000	-2.439438000	2.878018000
H	-0.283358000	-3.215264000	2.265534000
H	0.920236000	-2.928502000	3.544660000
H	0.733034000	-1.758782000	2.210052000
C	-1.711576000	4.481969000	-1.332491000
H	-2.320247000	5.112568000	-0.671285000
H	-1.279592000	5.132117000	-2.108621000
H	-0.891495000	4.052931000	-0.741817000
C	-3.444053000	-0.248547000	3.901601000
H	-2.961162000	0.629119000	4.360740000
C	-0.166722000	-0.628572000	4.631045000
H	0.337218000	0.136531000	4.028218000
H	0.588401000	-1.118297000	5.264153000
H	-0.884019000	-0.125349000	5.294197000
C	-5.428092000	4.069494000	-0.624107000
H	-4.834513000	4.910668000	-1.009077000
H	-6.241970000	4.492199000	-0.015590000
H	-5.885212000	3.546928000	-1.473211000
C	4.575282000	2.891957000	-2.031168000
H	5.393706000	2.335983000	-1.557177000
H	5.010813000	3.626107000	-2.725301000
H	3.980679000	2.183787000	-2.626616000

C	0.046911000	-3.420951000	-1.272106000
H	0.815178000	-3.935388000	-0.681565000
H	-0.733843000	-4.150772000	-1.532541000
H	-0.406521000	-2.643044000	-0.645495000
C	-3.838658000	-1.242540000	5.008192000
H	-4.298768000	-2.143521000	4.580386000
H	-4.577785000	-0.776865000	5.678296000
H	-2.982010000	-1.547945000	5.623549000
C	-4.023936000	3.848274000	1.485360000
H	-3.473441000	3.166299000	2.146340000
H	-4.856148000	4.281183000	2.061161000
H	-3.346068000	4.667867000	1.213093000
H	-1.307301000	2.336552000	1.335728000
H	-6.233938000	0.489234000	-4.366394000
H	-5.145881000	-3.517827000	-2.034536000
H	-3.437097000	-3.195189000	-2.319977000
H	-4.015879000	-5.525058000	2.133986000
H	4.820194000	-5.627637000	-1.103916000
H	6.428404000	-2.446340000	2.068412000
H	4.794507000	-2.247393000	2.705974000
H	7.355332000	2.178688000	2.755230000
H	-1.274044000	1.837383000	2.060935000

J(open-shell singlet)

Ti	-1.711103000	0.183477000	0.152266000
Ti	1.759201000	0.423416000	-0.706660000
P	-3.248107000	2.193108000	-0.459613000
P	2.570341000	-1.329574000	-2.417825000
P	3.016985000	2.414617000	0.336598000
P	-2.091507000	-1.291970000	2.162587000
N	3.356664000	-0.527090000	0.322473000
N	-3.568020000	-0.745502000	-0.316103000
N	0.028135000	-0.363134000	-0.504295000
N	0.136416000	0.837154000	0.267671000
C	3.754170000	-1.855053000	0.022803000
C	-4.640594000	1.271160000	-1.213006000
C	-4.799337000	-2.892126000	-0.466617000
C	3.917765000	-3.710797000	-1.591841000
H	3.694363000	-4.115875000	-2.578651000
C	-3.559227000	-3.756187000	1.899991000
H	-3.067940000	-4.101102000	2.809900000
C	4.012255000	0.074288000	1.425489000
C	-3.875224000	-2.033073000	0.182650000
C	-4.573029000	-0.151288000	-1.104518000
C	2.154416000	3.755303000	1.343220000
H	2.938057000	4.389537000	1.787278000
C	-6.618024000	-0.296279000	-2.437438000
H	-7.371964000	-0.914113000	-2.928591000
C	-3.263848000	-2.478725000	1.392149000
C	3.503981000	-2.405030000	-1.272661000
C	4.013239000	1.495695000	1.568444000
C	4.605761000	-4.498972000	-0.663125000
C	4.567104000	-2.189263000	2.385620000
C	4.694278000	-0.685184000	2.416081000
C	4.418290000	-2.685262000	0.967577000
C	5.402292000	1.348340000	3.574139000
C	-2.460038000	0.689487000	4.196221000
H	-1.542506000	0.499816000	4.768495000
H	-3.174715000	1.184521000	4.871031000
H	-2.210921000	1.385417000	3.382909000
C	-2.442378000	3.160291000	-1.882602000
H	-1.510914000	3.538180000	-1.432622000
C	-5.099860000	-4.144813000	0.082528000
H	-5.815452000	-4.786834000	-0.434232000
C	-4.062343000	3.519685000	0.611775000
H	-4.695175000	4.132304000	-0.049625000
C	5.391522000	-0.045981000	3.448130000
H	5.911299000	-0.662339000	4.183968000
C	-5.561361000	-0.926633000	-1.771952000
C	-0.717031000	-2.372188000	2.871476000
H	-1.177926000	-3.044160000	3.613094000
C	-4.480466000	-4.593012000	1.256627000
C	4.848337000	-3.968853000	0.609778000
H	5.361241000	-4.572507000	1.360839000
C	-2.062174000	2.164569000	-2.998718000
H	-1.466540000	1.323581000	-2.614335000
H	-1.465644000	2.673313000	-3.771113000
H	-2.961731000	1.752157000	-3.475153000
C	5.001815000	-0.069048000	-3.044963000
H	4.647668000	0.756928000	-2.413927000
H	5.688291000	0.343917000	-3.799118000
H	5.567951000	-0.758881000	-2.404873000
C	4.691385000	2.107006000	2.637987000
H	4.655699000	3.191053000	2.745627000
C	-5.380914000	-2.428760000	-1.784204000
C	4.332011000	3.307301000	-0.717524000
H	5.076437000	2.509727000	-0.868538000
C	-2.989981000	4.417065000	1.259097000
H	-2.310842000	3.821364000	1.885493000
H	-3.467724000	5.174148000	1.898669000
H	-2.382803000	4.944472000	0.510804000
C	-5.713513000	1.874598000	-1.897221000
H	-5.780584000	2.961252000	-1.938438000
C	1.388278000	-2.465419000	-3.341880000
H	1.997396000	-3.219134000	-3.865411000
C	1.324090000	3.122832000	2.479256000
H	0.563587000	2.445563000	2.072129000
H	0.823478000	3.920663000	3.049835000
H	1.956928000	2.553225000	3.170839000
C	-3.073196000	-0.615442000	3.648286000
H	-4.031790000	-0.361557000	3.168112000
C	0.354964000	-1.513979000	3.574903000
H	0.782835000	-0.778692000	2.881244000
H	1.169160000	-2.164034000	3.929509000
H	-0.043395000	-0.978696000	4.446053000
C	-3.348707000	-1.630261000	4.772103000
H	-3.838108000	-2.535206000	4.390705000
H	-4.014471000	-1.181698000	5.525323000
H	-2.422029000	-1.922927000	5.285907000
C	-6.714862000	1.101834000	-2.496320000
C	-3.226863000	4.352269000	-2.461175000
H	-4.145354000	4.019307000	-2.961519000
H	-2.609398000	4.865105000	-3.214588000
H	-3.495793000	5.092549000	-1.696235000
C	0.439085000	-3.189832000	-2.367420000
H	0.994162000	-3.808281000	-1.651171000
H	-0.236276000	-3.846634000	-2.936744000
H	-0.165267000	-2.470157000	-1.803104000
C	1.264222000	4.631473000	0.439226000
H	1.843631000	5.176015000	-0.317954000
H	0.733400000	5.375988000	1.051655000
H	0.516401000	4.012792000	-0.074333000
C	3.833022000	-0.800613000	-3.735225000
H	3.285916000	-0.072040000	-4.355569000
C	0.597068000	-1.655431000	-4.389731000
H	-0.008213000	-0.880973000	-3.899330000
H	-0.083273000	-2.322778000	-4.939188000
H	1.253021000	-1.167974000	-5.124862000
C	5.039112000	4.490660000	-0.032008000
H	4.346694000	5.323845000	0.153420000
H	5.843041000	4.869298000	-0.681446000
H	5.493905000	4.195895000	0.921611000
C	-4.962328000	2.860271000	1.673554000
H	-5.745338000	2.247251000	1.210005000
H	-5.446261000	3.635296000	2.286729000
H	-4.373353000	2.216222000	2.340363000
C	-0.078920000	-3.222096000	1.753751000
H	-0.813128000	-3.881483000	1.274216000

H	0.719221000	-3.848266000	2.180870000
H	0.360822000	-2.577190000	0.982867000
C	4.361461000	-1.926444000	-4.642213000
H	4.888607000	-2.689593000	-4.054010000
H	5.078284000	-1.510844000	-5.366842000
H	3.561842000	-2.416414000	-5.212978000
C	3.783257000	3.709186000	-2.103015000
H	3.317831000	2.856903000	-2.616472000
H	4.602085000	4.082900000	-2.736233000
H	3.030886000	4.505707000	-2.029197000
H	1.024021000	1.200318000	-2.361183000
H	5.934771000	1.830282000	4.392719000
H	5.425741000	-2.666634000	2.880829000
H	3.673110000	-2.487076000	2.967812000
H	4.931135000	-5.506120000	-0.919169000
H	-4.709221000	-5.577624000	1.662045000
H	-6.330227000	-2.940074000	-1.999847000
H	-4.686460000	-2.700847000	-2.603496000
H	-7.549294000	1.578356000	-3.008808000
H	1.077137000	1.845626000	-1.886727000

J(triplet)

Ti	-1.722953000	0.188589000	0.145053000
Ti	1.760324000	0.416084000	-0.696323000
P	-3.268499000	2.195792000	-0.447744000
P	2.580575000	-1.340835000	-2.412110000
P	3.016552000	2.430526000	0.322736000
P	-2.074808000	-1.312656000	2.146070000
N	3.368744000	-0.517980000	0.327591000
N	-3.583542000	-0.749851000	-0.310508000
N	0.025506000	-0.363271000	-0.508629000
N	0.145471000	0.840517000	0.262689000
C	3.768437000	-1.845730000	0.035106000
C	-4.673594000	1.271859000	-1.175257000
C	-4.811442000	-2.898723000	-0.461607000
C	3.931102000	-3.711666000	-1.567345000
H	3.705464000	-4.124351000	-2.550476000
C	-3.534851000	-3.780057000	1.878542000
H	-3.029994000	-4.131000000	2.778732000
C	4.022756000	0.094897000	1.423687000
C	-3.879307000	-2.042279000	0.180707000
C	-4.600976000	-0.151717000	-1.077980000
C	2.152752000	3.773759000	1.324519000
H	2.933773000	4.413882000	1.764709000
C	-6.669331000	-0.290601000	-2.376843000
H	-7.430041000	-0.906471000	-2.860029000
C	-3.248738000	-2.498070000	1.376765000
C	3.514963000	-2.404561000	-1.256206000
C	4.016131000	1.517594000	1.556782000
C	4.624918000	-4.491206000	-0.635744000
C	4.592150000	-2.159559000	2.396855000
C	4.712298000	-0.654465000	2.416943000
C	4.439038000	-2.666965000	0.983054000
C	5.414098000	1.390499000	3.558077000
C	-2.446511000	0.672445000	4.174158000
H	-1.528087000	0.483582000	4.745184000
H	-3.160808000	1.166716000	4.849979000
H	-2.198889000	1.369442000	3.361300000
C	-2.472201000	3.132807000	-1.896329000
H	-1.542524000	3.530542000	-1.459782000
C	-5.101546000	-4.156167000	0.081250000
H	-5.824209000	-4.794844000	-0.429860000
C	-4.063834000	3.545882000	0.607529000
H	-4.705827000	4.147025000	-0.055536000
C	5.410485000	-0.004818000	3.441529000
H	5.936914000	-0.613298000	4.179183000
C	-5.599556000	-0.923347000	-1.735638000
C	-0.701921000	-2.392525000	2.856695000
H	-1.161412000	-3.068860000	3.595226000
C	-4.464013000	-4.613302000	1.242423000
C	4.871660000	-3.951537000	0.632466000
H	5.389995000	-4.548380000	1.385230000
C	-2.087722000	2.111267000	-2.987519000
H	-1.476104000	1.289425000	-2.586495000
H	-1.505646000	2.606285000	-3.779734000
H	-2.985551000	1.673077000	-3.443772000
C	5.010377000	-0.076486000	-3.038790000
H	4.651291000	0.750158000	-2.411476000
H	5.696431000	0.336152000	-3.793487000
H	5.578116000	-0.761668000	-2.395138000
C	4.695163000	2.139091000	2.620116000
H	4.654142000	3.223571000	2.721038000
C	-5.414255000	-2.424610000	-1.765669000
C	4.325883000	3.319736000	-0.740117000
H	5.072311000	2.523465000	-0.887753000
C	-2.980567000	4.454408000	1.220162000
H	-2.292374000	3.871043000	1.848238000
H	-3.447381000	5.225329000	1.851231000
H	-2.384638000	4.965336000	0.451692000
C	-5.760165000	1.877771000	-1.835783000
H	-5.829965000	2.964664000	-1.867611000
C	1.404824000	-2.485176000	-3.333224000
H	2.015860000	-3.240206000	-3.852566000
C	1.325409000	3.142414000	2.463475000
H	0.571101000	2.456569000	2.059033000
H	0.817773000	3.940032000	3.028125000
H	1.961448000	2.582095000	3.159689000
C	-3.059334000	-0.632878000	3.626328000
H	-4.016360000	-0.378480000	3.143295000
C	0.366063000	-1.532948000	3.564621000
H	0.789986000	-0.791835000	2.874674000
H	1.183477000	-2.180872000	3.915758000
H	-0.034883000	-1.004415000	4.438760000
C	-3.338594000	-1.646700000	4.750000000
H	-3.824821000	-2.552639000	4.366680000
H	-4.008193000	-1.198635000	5.500067000
H	-2.413612000	-1.937943000	5.267719000
C	-6.770818000	1.107867000	-2.422441000
C	-3.270171000	4.301409000	-2.503070000
H	-4.188459000	3.945923000	-2.988068000
H	-2.661715000	4.798940000	-3.273906000
H	-3.541405000	5.059903000	-1.756883000
C	0.454836000	-3.205829000	-2.356761000
H	1.009417000	-3.822160000	-1.638320000
H	-0.220642000	-3.864218000	-2.924083000
H	-0.149081000	-2.483792000	-1.794902000
C	1.257821000	4.640906000	0.416345000
H	1.833901000	5.183095000	-0.345092000
H	0.724991000	5.387138000	1.024838000
H	0.511183000	4.016161000	-0.091807000
C	3.845764000	-0.815254000	-3.728293000
H	3.298570000	-0.091566000	-4.354306000
C	0.614026000	-1.680764000	-4.385908000
H	0.006128000	-0.905635000	-3.899704000
H	-0.064301000	-2.351435000	-4.933730000
H	1.270262000	-1.195214000	-5.122062000
C	5.030672000	4.510207000	-0.064632000
H	4.335840000	5.342200000	0.116973000
H	5.831544000	4.887114000	-0.718810000
H	5.488983000	4.223557000	0.889799000
C	-4.948793000	2.909243000	1.695838000
H	-5.738285000	2.286807000	1.256359000
H	-5.424188000	3.696872000	2.299536000
H	-4.350788000	2.279270000	2.368118000
C	-0.059058000	-3.234977000	1.735984000
H	-0.789554000	-3.896869000	1.254181000
H	0.743122000	-3.857906000	2.160252000
H	0.375939000	-2.584079000	0.967351000

C	4.379631000	-1.944896000	-4.627352000
H	4.905838000	-2.703964000	-4.033049000
H	5.098489000	-1.531897000	-5.351428000
H	3.583048000	-2.439321000	-5.198525000
C	3.771490000	3.709483000	-2.126849000
H	3.307802000	2.851244000	-2.631958000
H	4.586908000	4.081121000	-2.765591000
H	3.016786000	4.504179000	-2.056705000
H	1.030612000	1.208144000	-2.369550000
H	5.947417000	1.880861000	4.371063000
H	5.455347000	-2.629331000	2.891412000
H	3.702346000	-2.457451000	2.985331000
H	4.952194000	-5.499141000	-0.886148000
H	-4.685156000	-5.601623000	1.643008000
H	-6.364723000	-2.937383000	-1.972598000
H	-4.730741000	-2.685707000	-2.597724000
H	-7.615651000	1.586533000	-2.915535000
H	1.055835000	1.839641000	-1.887540000

TS$_{JK}$(closed-shell singlet)

Ti	1.752908000	0.266034000	-0.398591000
Ti	-1.709397000	0.445230000	0.307009000
P	2.996101000	2.438523000	-0.064251000
P	-2.331740000	-0.798033000	2.451941000
P	-3.478100000	2.132528000	-0.486780000
P	2.172775000	-1.902387000	-1.725766000
N	-3.144683000	-0.829571000	-0.318283000
N	3.737594000	-0.422454000	0.274146000
N	0.257609000	0.344057000	0.693251000
N	-0.065338000	0.789331000	-0.663417000
C	-3.352209000	-2.104678000	0.246803000
C	4.578400000	1.867203000	0.646207000
C	5.190072000	-2.321253000	0.986160000
C	-3.157025000	-3.573016000	2.185984000
H	-2.863356000	-3.741978000	3.221845000
C	3.919682000	-3.992295000	-0.871795000
H	3.412103000	-4.643209000	-1.583951000
C	-3.960653000	-0.473049000	-1.409994000
C	4.145735000	-1.774910000	0.188962000
C	4.687797000	0.456336000	0.847397000
C	-2.920790000	3.550997000	-1.620699000
H	-3.816476000	3.953660000	-2.119151000
C	6.797908000	0.879827000	2.024537000
H	7.640482000	0.483679000	2.594367000
C	3.516668000	-2.651151000	-0.748798000
C	-2.988800000	-2.301638000	1.609089000
C	-4.202797000	0.911108000	-1.667503000
C	-3.715808000	-4.626379000	1.445323000
C	-4.250229000	-2.919547000	-1.960063000
C	-4.564473000	-1.459213000	-2.229069000
C	-3.925296000	-3.159771000	-0.497606000
C	-5.596888000	0.293409000	-3.580164000
C	2.212432000	-0.434865000	-4.182129000
H	1.282368000	-0.852805000	-4.586825000
H	2.815199000	-0.078227000	-5.030692000
H	1.940472000	0.438047000	-3.570711000
C	2.197806000	3.574239000	1.228338000
H	1.171203000	3.694641000	0.848025000
C	5.590702000	-3.652625000	0.823681000
H	6.398654000	-4.031993000	1.451913000
C	3.490763000	3.591396000	-1.478441000
H	4.106334000	4.396666000	-1.047595000
C	-5.390815000	-1.062941000	-3.288706000
H	-5.863167000	-1.829336000	-3.905472000
C	5.793185000	-0.005355000	1.618334000
C	0.934384000	-3.278626000	-2.037033000
H	1.479099000	-4.107009000	-2.516797000
C	4.964859000	-4.503968000	-0.095340000
C	-4.109188000	-4.407816000	0.118145000
H	-4.548289000	-5.223086000	-0.459479000
C	2.126627000	2.840510000	2.582688000
H	1.628861000	1.869295000	2.477110000
H	1.557033000	3.448086000	3.302002000
H	3.133256000	2.679394000	2.991855000
C	-5.072026000	-0.244569000	2.817243000
H	-4.920640000	0.297996000	1.874864000
H	-5.856242000	0.266588000	3.395532000
H	-5.430194000	-1.252782000	2.568829000
C	-4.995035000	1.269475000	-2.777038000
H	-5.155059000	2.322101000	-3.008318000
C	5.798838000	-1.449610000	2.057206000
C	-5.006992000	2.847724000	0.425835000
H	-5.600050000	1.937678000	0.601815000
C	2.240503000	4.203976000	-2.138141000
H	1.581340000	3.415655000	-2.527819000
H	2.534560000	4.852558000	-2.976963000
H	1.653969000	4.809607000	-1.434235000
C	5.602406000	2.734311000	1.070054000
H	5.517508000	3.800759000	0.863174000
C	-1.024909000	-1.431620000	3.657128000
H	-1.532642000	-2.107975000	4.361950000
C	-1.944045000	3.027056000	-2.691517000
H	-1.068634000	2.559799000	-2.220306000
H	-1.601356000	3.864989000	-3.318800000
H	-2.419579000	2.283609000	-3.343415000
C	3.012623000	-1.479862000	-3.374688000
H	3.942909000	-1.001188000	-3.028850000
C	-0.199177000	-2.822951000	-2.978372000
H	-0.711566000	-1.936951000	-2.581262000
H	-0.938532000	-3.632143000	-3.070631000
H	0.164260000	-2.591418000	-3.987396000
C	3.392311000	-2.703990000	-4.226750000
H	4.002706000	-3.415554000	-3.656134000
H	3.978020000	-2.383407000	-5.101389000
H	2.501013000	-3.227899000	-4.599860000
C	6.732978000	2.249386000	1.736105000
C	2.831076000	4.968696000	1.396435000
H	3.847208000	4.896909000	1.805631000
H	2.230727000	5.552659000	2.110465000
H	2.872297000	5.536726000	0.458111000
C	0.090563000	-2.219354000	2.946492000
H	-0.307053000	-3.108149000	2.440517000
H	0.833724000	-2.553028000	3.687549000
H	0.597687000	-1.595022000	2.201125000
C	-2.265026000	4.680736000	-0.802064000
H	-2.953092000	5.127669000	-0.072676000
H	-1.925540000	5.481939000	-1.475886000
H	-1.387081000	4.303863000	-0.258734000
C	-3.767746000	-0.320715000	3.632314000
H	-3.501257000	0.698192000	3.958280000
C	-0.445572000	-0.240111000	4.448579000
H	0.062017000	0.458356000	3.770954000
H	0.290287000	-0.598969000	5.184031000
H	-1.221864000	0.314422000	4.994912000
C	-5.878263000	3.834739000	-0.371721000
H	-5.347901000	4.775704000	-0.573644000
H	-6.779124000	4.084791000	0.210067000
H	-6.210344000	3.409741000	-1.327233000
C	4.347077000	2.825630000	-2.505341000
H	5.246396000	2.399999000	-2.042542000
H	4.660489000	3.502690000	-3.314010000
H	3.774342000	2.005151000	-2.961267000
C	0.366001000	-3.766716000	-0.688768000
H	1.157825000	-4.128851000	-0.021513000
H	-0.344448000	-4.588007000	-0.862310000
H	-0.171959000	-2.958646000	-0.177198000
C	-3.967466000	-1.205818000	4.876222000
H	-4.170095000	-2.247765000	4.591118000

H	-4.837235000	-0.847290000	5.448983000
H	-3.101738000	-1.191401000	5.550947000
C	-4.611324000	3.424690000	1.799374000
H	-3.991280000	2.713808000	2.361817000
H	-5.513583000	3.640850000	2.391230000
H	-4.047237000	4.362416000	1.700562000
H	-1.028194000	2.994202000	1.813208000
H	-6.225437000	0.585807000	-4.420337000
H	-5.087870000	-3.557301000	-2.280640000
H	-3.384546000	-3.222802000	-2.579386000
H	-3.851888000	-5.605553000	1.903021000
H	5.278296000	-5.541655000	-0.197830000
H	6.816125000	-1.784256000	2.307693000
H	5.203790000	-1.545643000	2.986959000
H	7.529295000	2.923677000	2.047370000
H	-1.459426000	2.451944000	2.093846000

TS$_{JK}$(open-shell singlet)

Ti	-1.752501000	0.138492000	0.098468000
Ti	1.779470000	0.323402000	-0.505643000
P	-3.194754000	2.213269000	-0.388967000
P	2.659305000	-1.141785000	-2.449924000
P	3.135951000	2.336295000	0.460448000
P	-2.262210000	-1.381459000	2.098920000
N	3.382138000	-0.630640000	0.373012000
N	-3.641811000	-0.706418000	-0.409979000
N	-0.011695000	-0.378680000	-0.572811000
N	0.045592000	0.762406000	0.326598000
C	3.783618000	-1.924063000	-0.033282000
C	-4.635446000	1.394152000	-1.180855000
C	-4.952897000	-2.790690000	-0.658347000
C	3.952169000	-3.622748000	-1.794429000
H	3.745174000	-3.946098000	-2.814258000
C	-3.770274000	-3.798674000	1.683172000
H	-3.304523000	-4.198423000	2.584058000
C	4.032640000	-0.090362000	1.504236000
C	-4.001209000	-1.996314000	0.034442000
C	-4.625694000	-0.032034000	-1.158157000
C	2.299319000	3.677733000	1.491289000
H	3.087124000	4.256825000	1.998589000
C	-6.675595000	-0.028353000	-2.486204000
H	-7.453378000	-0.587264000	-3.009654000
C	-3.425541000	-2.510609000	1.234720000
C	3.546363000	-2.342504000	-1.377111000
C	4.042946000	1.323839000	1.702998000
C	4.622366000	-4.488217000	-0.920439000
C	4.572937000	-2.417490000	2.306533000
C	4.695531000	-0.915712000	2.450176000
C	4.435255000	-2.818584000	0.853855000
C	5.377402000	1.048168000	3.732867000
C	-2.636924000	0.509136000	4.211806000
H	-1.754356000	0.253911000	4.812669000
H	-3.361755000	0.997738000	4.880147000
H	-2.326506000	1.233902000	3.446930000
C	-2.374141000	3.222229000	-1.780037000
H	-1.399070000	3.496157000	-1.346514000
C	-5.304899000	-4.051698000	-0.164738000
H	-6.041495000	-4.643436000	-0.711113000
C	-3.959578000	3.531246000	0.735997000
H	-4.547501000	4.211029000	0.099648000
C	5.374138000	-0.337824000	3.529908000
H	5.885390000	-0.992094000	4.238229000
C	-5.641996000	-0.734042000	-1.860633000
C	-0.922087000	-2.511713000	2.794015000
H	-1.406912000	-3.203202000	3.501698000
C	-4.711608000	-4.573126000	0.994024000
C	4.861717000	-4.071563000	0.395194000
H	5.367761000	-4.740648000	1.093382000
C	-2.119806000	2.290739000	-2.983665000
H	-1.571650000	1.384382000	-2.688657000
H	-1.523514000	2.813829000	-3.746328000
H	-3.068600000	1.981020000	-3.441758000
C	5.189902000	-0.005928000	-2.903178000
H	4.879800000	0.702086000	-2.124114000
H	5.884867000	0.505960000	-3.585294000
H	5.730099000	-0.827674000	-2.414039000
C	4.695942000	1.866988000	2.824311000
H	4.673592000	2.943768000	2.990206000
C	-5.510551000	-2.239419000	-1.952981000
C	4.537424000	3.209552000	-0.493075000
H	5.254548000	2.386146000	-0.634291000
C	-2.848216000	4.332586000	1.440865000
H	-2.214476000	3.667603000	2.044655000
H	-3.289712000	5.085599000	2.110896000
H	-2.198317000	4.857518000	0.727263000
C	-5.686482000	2.074187000	-1.825243000
H	-5.713855000	3.163204000	-1.805939000
C	1.492092000	-2.183500000	-3.499084000
H	2.107034000	-2.878608000	-4.091985000
C	1.384216000	3.037144000	2.555304000
H	0.624078000	2.402010000	2.083068000
H	0.878712000	3.831596000	3.126160000
H	1.956377000	2.421176000	3.260256000
C	-3.275611000	-0.742285000	3.574548000
H	-4.204304000	-0.428813000	3.071802000
C	0.151706000	-1.697620000	3.546091000
H	0.590256000	-0.933946000	2.890507000
H	0.957172000	-2.370864000	3.876520000
H	-0.249760000	-1.199558000	4.437531000
C	-3.629608000	-1.801916000	4.633051000
H	-4.136074000	-2.667384000	4.187805000
H	-4.307001000	-1.366357000	5.383311000
H	-2.734077000	-2.154270000	5.164313000
C	-6.717152000	1.373441000	-2.464093000
C	-3.086146000	4.509997000	-2.234814000
H	-4.055145000	4.287649000	-2.700505000
H	-2.469034000	5.020060000	-2.990542000
H	-3.250032000	5.217445000	-1.411686000
C	0.528411000	-3.002823000	-2.618673000
H	1.072215000	-3.700689000	-1.969544000
H	-0.145178000	-3.588365000	-3.263183000
H	-0.075954000	-2.343556000	-1.984664000
C	1.494081000	4.631068000	0.584691000
H	2.131160000	5.168200000	-0.130139000
H	0.978300000	5.382114000	1.201755000
H	0.733210000	4.074235000	0.021033000
C	3.977317000	-0.544928000	-3.686640000
H	3.491886000	0.301346000	-4.199684000
C	0.714476000	-1.263531000	-4.464021000
H	0.096129000	-0.552891000	-3.899170000
H	0.047239000	-1.866074000	-5.098039000
H	1.379943000	-0.692555000	-5.127323000
C	5.254699000	4.338306000	0.269462000
H	4.589206000	5.194580000	0.447793000
H	6.106566000	4.702313000	-0.324884000
H	5.646769000	3.994011000	1.234474000
C	-4.910444000	2.874147000	1.753221000
H	-5.725906000	2.338479000	1.251264000
H	-5.351078000	3.642998000	2.405867000
H	-4.370989000	2.158368000	2.388064000
C	-0.278011000	-3.331002000	1.655992000
H	-1.011175000	-3.969266000	1.147251000
H	0.510075000	-3.976679000	2.072560000
H	0.175399000	-2.666116000	0.909524000
C	4.428723000	-1.572442000	-4.740511000
H	4.884789000	-2.450829000	-4.263791000
H	5.189410000	-1.119160000	-5.394522000
H	3.603568000	-1.911640000	-5.380059000

C	4.073869000	3.674359000	-1.888885000
H	3.591814000	2.856512000	-2.440217000
H	4.939114000	4.022351000	-2.472980000
H	3.360036000	4.506774000	-1.826336000
H	1.199504000	1.876489000	-2.638867000
H	5.893783000	1.481778000	4.588005000
H	5.429631000	-2.925693000	2.773451000
H	3.675912000	-2.758429000	2.859520000
H	4.944801000	-5.472580000	-1.256629000
H	-4.979701000	-5.565434000	1.353822000
H	-6.473804000	-2.708276000	-2.200406000
H	-4.818355000	-2.489142000	-2.781112000
H	-7.533153000	1.910055000	-2.946133000
H	0.770575000	2.417796000	-2.358767000

TS_{JK}(triplet)

Ti	-1.737390000	0.112389000	0.025883000
Ti	1.761858000	0.337120000	-0.586745000
P	-3.262082000	2.180091000	-0.442049000
P	2.645634000	-1.264497000	-2.406288000
P	3.084506000	2.407254000	0.358664000
P	-2.132153000	-1.304261000	2.086226000
N	3.379953000	-0.569843000	0.366688000
N	-3.641544000	-0.754874000	-0.370800000
N	0.019161000	-0.444502000	-0.555565000
N	0.031864000	0.789644000	0.252842000
C	3.811763000	-1.875165000	0.029699000
C	-4.705685000	1.305227000	-1.164344000
C	-4.929330000	-2.864781000	-0.479950000
C	4.033629000	-3.659092000	-1.644688000
H	3.836999000	-4.036318000	-2.648007000
C	-3.623580000	-3.761720000	1.841573000
H	-3.112885000	-4.118560000	2.736069000
C	3.989103000	0.022058000	1.495103000
C	-3.959972000	-2.033171000	0.137456000
C	-4.668654000	-0.120012000	-1.093188000
C	2.217147000	3.784048000	1.312154000
H	2.990217000	4.392415000	1.807498000
C	-6.777673000	-0.196248000	-2.323195000
H	-7.569850000	-0.785668000	-2.788319000
C	-3.320152000	-2.487967000	1.328359000
C	3.590209000	-2.372893000	-1.290095000
C	3.963747000	1.442843000	1.652978000
C	4.721319000	-4.464608000	-0.728293000
C	4.578380000	-2.257955000	2.399147000
C	4.650794000	-0.750079000	2.488438000
C	4.473588000	-2.716235000	0.962136000
C	5.247220000	1.269976000	3.727178000
C	-2.468619000	0.684545000	4.116586000
H	-1.575399000	0.462620000	4.714949000
H	-3.183284000	1.205972000	4.771211000
H	-2.172172000	1.368255000	3.309541000
C	-2.476963000	3.119629000	-1.895690000
H	-1.534298000	3.499426000	-1.470850000
C	-5.237318000	-4.111649000	0.076865000
H	-5.987511000	-4.735954000	-0.411638000
C	-4.014921000	3.540691000	0.633328000
H	-4.643665000	4.164056000	-0.021709000
C	5.284066000	-0.120873000	3.566384000
H	5.792086000	-0.740393000	4.307633000
C	-5.704089000	-0.862963000	-1.723897000
C	-0.769688000	-2.388940000	2.808261000
H	-1.235836000	-3.039654000	3.565581000
C	-4.582534000	-4.576738000	1.225924000
C	4.934400000	-3.978922000	0.567565000
H	5.446510000	-4.601350000	1.303640000
C	-2.125563000	2.095848000	-2.995306000
H	-1.490286000	1.283096000	-2.610838000
H	-1.573567000	2.587841000	-3.810122000
H	-3.035504000	1.649506000	-3.418736000
C	5.114555000	-0.047654000	-2.968500000
H	4.782664000	0.703495000	-2.240060000
H	5.784483000	0.440255000	-3.692110000
H	5.689898000	-0.809228000	-2.425052000
C	4.571549000	2.039014000	2.773414000
H	4.518235000	3.119929000	2.901528000
C	-5.553112000	-2.369126000	-1.767261000
C	4.507297000	3.236388000	-0.599322000
H	5.212583000	2.398555000	-0.713784000
C	-2.902890000	4.415658000	1.243267000
H	-2.227929000	3.810914000	1.864881000
H	-3.344393000	5.197175000	1.879582000
H	-2.297512000	4.912523000	0.472902000
C	-5.797686000	1.944540000	-1.782883000
H	-5.844901000	3.032931000	-1.798850000
C	1.494716000	-2.395638000	-3.377261000
H	2.120168000	-3.104947000	-3.941756000
C	1.287385000	3.182867000	2.386721000
H	0.548309000	2.511705000	1.931090000
H	0.758266000	3.997399000	2.905526000
H	1.852337000	2.611817000	3.133692000
C	-3.113696000	-0.599550000	3.555735000
H	-4.055002000	-0.314823000	3.058885000
C	0.315863000	-1.528717000	3.488609000
H	0.733964000	-0.800312000	2.781831000
H	1.132875000	-2.178805000	3.836485000
H	-0.067830000	-0.984732000	4.360819000
C	-3.439151000	-1.607331000	4.672379000
H	-3.948260000	-2.496914000	4.280715000
H	-4.104047000	-1.139849000	5.414730000
H	-2.530499000	-1.927972000	5.201603000
C	-6.843426000	1.204971000	-2.348215000
C	-3.265479000	4.303038000	-2.485318000
H	-4.195506000	3.964051000	-2.959779000
H	-2.660538000	4.796198000	-3.261771000
H	-3.515225000	5.061468000	-1.731539000
C	0.570796000	-3.192077000	-2.435664000
H	1.145595000	-3.841861000	-1.763904000
H	-0.101486000	-3.826287000	-3.033920000
H	-0.036582000	-2.515569000	-1.822861000
C	1.421858000	4.689884000	0.349515000
H	2.068764000	5.204351000	-0.372995000
H	0.885884000	5.460113000	0.924239000
H	0.679028000	4.102210000	-0.206740000
C	3.919002000	-0.690090000	-3.698793000
H	3.390382000	0.098761000	-4.258753000
C	0.674685000	-1.553596000	-4.377075000
H	0.046492000	-0.829520000	-3.840748000
H	0.014555000	-2.208930000	-4.964549000
H	1.312712000	-1.002154000	-5.082427000
C	5.232063000	4.369121000	0.149892000
H	4.577585000	5.239343000	0.299797000
H	6.098062000	4.706723000	-0.439460000
H	5.603885000	4.038498000	1.127501000
C	-4.911528000	2.924261000	1.723194000
H	-5.721732000	2.327769000	1.285334000
H	-5.360601000	3.722733000	2.332881000
H	-4.328979000	2.274675000	2.389694000
C	-0.145646000	-3.269547000	1.705927000
H	-0.888442000	-3.930070000	1.241292000
H	0.645320000	-3.896636000	2.145010000
H	0.299045000	-2.644600000	0.921483000
C	4.406379000	-1.760793000	-4.691723000
H	4.909840000	-2.584191000	-4.167143000
H	5.135968000	-1.315429000	-5.385515000
H	3.590303000	-2.178900000	-5.295214000
C	4.071581000	3.681665000	-2.010566000
H	3.581001000	2.864654000	-2.554822000

H	4.951778000	4.000383000	-2.588890000
H	3.374958000	4.530023000	-1.974672000
H	1.297828000	1.705085000	-2.913940000
H	5.728403000	1.743833000	4.581450000
H	5.444396000	-2.720122000	2.896089000
H	3.685566000	-2.608074000	2.953145000
H	5.071392000	-5.455380000	-1.014284000
H	-4.817381000	-5.557814000	1.636370000
H	-6.519345000	-2.859414000	-1.953925000
H	-4.895132000	-2.639416000	-2.616593000
H	-7.690440000	1.710603000	-2.809673000
H	0.950351000	2.364655000	-2.949539000

K(closed-shell singlet)

Ti	-1.799610000	-0.065630000	0.065128000
Ti	1.768469000	0.072734000	-0.289508000
P	-3.088431000	2.134967000	-0.367791000
P	2.832736000	-0.663007000	-2.482929000
P	2.962143000	2.073116000	0.838998000
P	-2.518909000	-1.408298000	2.081214000
N	3.496953000	-0.743176000	0.408182000
N	-3.626821000	-0.721246000	-0.597343000
N	-0.004769000	-0.624851000	-0.277079000
N	-0.037806000	0.791070000	0.000238000
C	3.974098000	-1.895197000	-0.246100000
C	-4.443573000	1.427418000	-1.400569000
C	-4.990029000	-2.742239000	-0.949999000
C	4.136343000	-3.229265000	-2.289059000
H	3.905166000	-3.380901000	-3.343063000
C	-4.046889000	-3.780963000	1.490094000
H	-3.681839000	-4.195691000	2.429402000
C	4.225716000	-0.292700000	1.522289000
C	-4.071698000	-1.990624000	-0.174825000
C	-4.511400000	0.006443000	-1.416094000
C	2.029116000	3.097733000	2.124074000
H	2.773180000	3.687306000	2.682689000
C	-6.402954000	0.113912000	-2.939676000
H	-7.153199000	-0.396775000	-3.545674000
C	-3.622662000	-2.501345000	1.080515000
C	3.696643000	-2.059465000	-1.637974000
C	4.122166000	1.079704000	1.882580000
C	4.896210000	-4.187972000	-1.606978000
C	5.013397000	-2.648007000	1.918037000
C	5.047051000	-1.170575000	2.267472000
C	4.753367000	-2.860180000	0.437706000
C	5.680696000	0.685263000	3.721466000
C	-3.036991000	0.413996000	4.221024000
H	-2.240528000	0.104997000	4.911106000
H	-3.808514000	0.924432000	4.816616000
H	-2.612422000	1.137238000	3.511309000
C	-2.091444000	3.259470000	-1.536074000
H	-1.183798000	3.471365000	-0.950629000
C	-5.431268000	-3.986939000	-0.485493000
H	-6.144876000	-4.553321000	-1.086023000
C	-4.007708000	3.367387000	0.747168000
H	-4.506356000	4.094208000	0.086867000
C	5.780839000	-0.662734000	3.348518000
H	6.417441000	-1.338751000	3.921810000
C	-5.480646000	-0.649914000	-2.212883000
C	-1.297103000	-2.608056000	2.889204000
H	-1.870856000	-3.257148000	3.569630000
C	-4.951428000	-4.521852000	0.719204000
C	5.217768000	-3.984487000	-0.256236000
H	5.824753000	-4.720293000	0.273716000
C	-1.661849000	2.445138000	-2.772754000
H	-1.131401000	1.530383000	-2.476503000
H	-0.976768000	3.041141000	-3.394705000
H	-2.530124000	2.168472000	-3.386500000
C	5.390565000	0.514118000	-2.554052000
H	5.044141000	0.997611000	-1.632388000
H	6.102141000	1.185576000	-3.056971000
H	5.924831000	-0.402769000	-2.270915000
C	4.841288000	1.545596000	2.997584000
H	4.749936000	2.586090000	3.308034000
C	-5.421835000	-2.163916000	-2.283867000
C	4.115631000	3.331133000	-0.029981000
H	4.966742000	2.693901000	-0.314099000
C	-3.012917000	4.110709000	1.657648000
H	-2.461377000	3.401075000	2.290439000
H	-3.550671000	4.809044000	2.316617000
H	-2.276786000	4.689242000	1.083483000
C	-5.381868000	2.163559000	-2.147563000
H	-5.364852000	3.251988000	-2.114879000
C	1.766108000	-1.473699000	-3.813693000
H	2.442175000	-2.022922000	-4.487072000
C	1.288651000	2.170271000	3.107552000
H	0.534920000	1.576683000	2.573109000
H	0.774213000	2.775732000	3.870055000
H	1.978356000	1.488822000	3.622108000
C	-3.653393000	-0.793727000	3.486555000
H	-4.517446000	-0.432170000	2.907087000
C	-0.236915000	-1.843229000	3.709121000
H	0.314153000	-1.140890000	3.069247000
H	0.488206000	-2.555590000	4.130557000
H	-0.673028000	-1.279393000	4.542771000
C	-4.144325000	-1.867552000	4.473434000
H	-4.638237000	-2.700170000	3.957345000
H	-4.873871000	-1.426363000	5.169907000
H	-3.317915000	-2.269348000	5.076919000
C	-6.365604000	1.515433000	-2.908309000
C	-2.726704000	4.596765000	-1.961487000
H	-3.613276000	4.439440000	-2.589868000
H	-2.001187000	5.169842000	-2.559340000
H	-3.014768000	5.222433000	-1.106952000
C	0.761418000	-2.469236000	-3.203386000
H	1.272303000	-3.286362000	-2.678190000
H	0.146458000	-2.907683000	-4.004322000
H	0.099778000	-1.967734000	-2.485624000
C	1.033691000	4.057954000	1.444232000
H	1.532445000	4.791256000	0.797137000
H	0.472130000	4.615450000	2.209427000
H	0.316418000	3.488696000	0.839743000
C	4.214947000	0.187708000	-3.493759000
H	3.754223000	1.134767000	-3.818389000
C	1.041966000	-0.381668000	-4.629376000
H	0.364418000	0.197440000	-3.987778000
H	0.439213000	-0.845367000	-5.424271000
H	1.742100000	0.318790000	-5.105824000
C	4.657480000	4.478324000	0.842488000
H	3.856076000	5.153029000	1.173761000
H	5.372974000	5.079998000	0.260792000
H	5.185306000	4.104694000	1.728814000
C	-5.085448000	2.640553000	1.570680000
H	-5.826988000	2.155902000	0.923207000
H	-5.609749000	3.358482000	2.219674000
H	-4.633629000	1.870346000	2.209481000
C	-0.608482000	-3.484102000	1.822579000
H	-1.328920000	-4.092002000	1.261923000
H	0.104889000	-4.162920000	2.314630000
H	-0.056430000	-2.858223000	1.109375000
C	4.712244000	-0.580704000	-4.731919000
H	5.120452000	-1.560899000	-4.448802000
H	5.522243000	-0.013653000	-5.216153000
H	3.924555000	-0.733887000	-5.480815000
C	3.470340000	3.858336000	-1.327292000
H	3.087506000	3.030219000	-1.939567000
H	4.211661000	4.418267000	-1.917543000
H	2.631302000	4.536113000	-1.117965000

H	6.244655000	1.061060000	4.574215000
H	5.947027000	-3.143815000	2.222248000
H	4.205120000	-3.133101000	2.499223000
H	5.248153000	-5.078225000	-2.126409000
H	-5.286594000	-5.501134000	1.058130000
H	-6.389393000	-2.582336000	-2.596533000
H	-4.689476000	-2.458613000	-3.060547000
H	-7.093007000	2.096922000	-3.473260000

K(open-shell singlet)

Ti	-1.656727000	0.209036000	0.440069000
Ti	1.736205000	-0.024929000	-0.028751000
P	-2.662545000	2.111964000	-1.017889000
P	2.201352000	-1.800561000	-1.863297000
P	3.031415000	2.239684000	0.230375000
P	-2.890008000	-0.614569000	2.540634000
N	3.664656000	-0.666041000	0.465536000
N	-3.405557000	-0.677871000	-0.373506000
N	-0.003933000	-0.726747000	0.382778000
N	0.164797000	0.650703000	0.905743000
C	4.101161000	-1.977226000	0.160215000
C	-3.853320000	1.099721000	-1.990300000
C	-4.813071000	-2.710971000	-0.422696000
C	3.990748000	-3.963464000	-1.280096000
H	3.540248000	-4.492707000	-2.119340000
C	-4.484293000	-2.996538000	2.353171000
H	-4.344614000	-3.119628000	3.427254000
C	4.546836000	0.125224000	1.234429000
C	-4.020461000	-1.764298000	0.280635000
C	-4.026003000	-0.249496000	-1.560729000
C	2.365461000	3.609566000	1.342382000
H	3.170415000	4.347777000	1.485760000
C	-5.557224000	-0.612429000	-3.428240000
H	-6.201568000	-1.287950000	-3.993789000
C	-3.879007000	-1.910158000	1.694662000
C	3.542999000	-2.669546000	-0.957619000
C	4.428610000	1.548035000	1.208366000
C	5.006805000	-4.582698000	-0.542529000
C	5.594353000	-1.956450000	2.185650000
C	5.569506000	-0.451991000	2.034692000
C	5.102472000	-2.631794000	0.925420000
C	6.356798000	1.763143000	2.696899000
C	-3.614862000	1.805929000	3.876047000
H	-2.957204000	1.706928000	4.749451000
H	-4.435534000	2.483377000	4.155449000
H	-3.036938000	2.277226000	3.069168000
C	-1.400190000	2.775672000	-2.279941000
H	-0.606547000	3.189982000	-1.639860000
C	-5.436808000	-3.755149000	0.268326000
H	-6.045899000	-4.466349000	-0.292471000
C	-3.678598000	3.645148000	-0.550609000
H	-4.015560000	4.114402000	-1.488196000
C	6.468637000	0.366966000	2.726551000
H	7.251985000	-0.103259000	3.323573000
C	-4.860164000	-1.111164000	-2.322222000
C	-1.902151000	-1.529180000	3.862254000
H	-2.619088000	-1.949963000	4.585411000
C	-5.270251000	-3.918034000	1.651395000
C	5.554226000	-3.903554000	0.553290000
H	6.331678000	-4.378679000	1.154155000
C	-0.800582000	1.592421000	-3.065426000
H	-0.363494000	0.842623000	-2.389753000
H	-0.003527000	1.952365000	-3.733659000
H	-1.566974000	1.099237000	-3.678950000
C	4.205362000	-0.452517000	-3.293771000
H	3.975507000	0.389832000	-2.628833000
H	4.578361000	-0.051791000	-4.248090000
H	5.009623000	-1.039074000	-2.829466000
C	5.321377000	2.340333000	1.953092000
H	5.204295000	3.423694000	1.955451000
C	-4.897878000	-2.572492000	-1.927919000
C	3.887919000	3.092942000	-1.239201000
H	4.629120000	2.334331000	-1.535303000
C	-2.812492000	4.646875000	0.235302000
H	-2.426855000	4.186734000	1.156568000
H	-3.410932000	5.525562000	0.519377000
H	-1.952277000	5.001103000	-0.348811000
C	-4.568009000	1.568716000	-3.109020000
H	-4.472686000	2.610997000	-3.409917000
C	0.949248000	-3.143990000	-2.275524000
H	1.463936000	-3.900217000	-2.889008000
C	1.966481000	3.026674000	2.714621000
H	1.200665000	2.249807000	2.591202000
H	1.554987000	3.830294000	3.344699000
H	2.827099000	2.590207000	3.236387000
C	-4.189084000	0.442610000	3.437496000
H	-4.910722000	0.624873000	2.625535000
C	-0.951504000	-0.560126000	4.597556000
H	-0.276382000	-0.070057000	3.883248000
H	-0.340245000	-1.123337000	5.318604000
H	-1.490835000	0.216147000	5.154903000
C	-4.924773000	-0.260675000	4.592066000
H	-5.390608000	-1.198507000	4.264994000
H	-5.722124000	0.392867000	4.977430000
H	-4.245707000	-0.478954000	5.428442000
C	-5.429665000	0.726898000	-3.823722000
C	-1.871352000	3.882424000	-3.243179000
H	-2.619306000	3.506628000	-3.952983000
H	-1.011974000	4.237511000	-3.832664000
H	-2.293419000	4.750934000	-2.721160000
C	0.429405000	-3.818984000	-0.990377000
H	1.241619000	-4.304956000	-0.434680000
H	-0.311515000	-4.588275000	-1.256455000
H	-0.049952000	-3.084596000	-0.331934000
C	1.156697000	4.306128000	0.687807000
H	1.414908000	4.790497000	-0.263455000
H	0.767939000	5.083709000	1.362643000
H	0.355335000	3.577914000	0.507541000
C	2.961507000	-1.329023000	-3.537114000
H	2.185755000	-0.706018000	-4.010682000
C	-0.211473000	-2.544955000	-3.096586000
H	-0.745320000	-1.785824000	-2.510194000
H	-0.927474000	-3.338390000	-3.358319000
H	0.131712000	-2.083017000	-4.033120000
C	4.641811000	4.392824000	-0.904666000
H	3.954062000	5.188625000	-0.586077000
H	5.170766000	4.753722000	-1.799760000
H	5.389171000	4.240420000	-0.116515000
C	-4.921787000	3.227281000	0.255950000
H	-5.565417000	2.551555000	-0.320958000
H	-5.509256000	4.117176000	0.528404000
H	-4.632242000	2.714567000	1.183356000
C	-1.097014000	-2.681460000	3.225327000
H	-1.750857000	-3.424131000	2.751798000
H	-0.510021000	-3.187299000	4.007011000
H	-0.407117000	-2.295199000	2.463296000
C	3.297556000	-2.504059000	-4.473121000
H	4.049039000	-3.164989000	-4.020471000
H	3.719286000	-2.116845000	-5.413210000
H	2.414325000	-3.103441000	-4.729463000
C	2.916441000	3.291401000	-2.420812000
H	2.381230000	2.361844000	-2.655843000
H	3.474474000	3.608135000	-3.314882000
H	2.168606000	4.066549000	-2.205331000
H	7.052003000	2.387772000	3.255761000
H	6.601605000	-2.308150000	2.452892000
H	4.934267000	-2.242942000	3.027856000
H	5.356069000	-5.579191000	-0.808674000

H	-5.744283000	-4.749033000	2.171624000
H	-5.799364000	-3.065820000	-2.319215000
H	-4.033571000	-3.091049000	-2.387635000
H	-5.986523000	1.106211000	-4.679438000

K(triplet)

Ti	-1.625308000	0.216521000	0.438546000
Ti	1.713844000	-0.043261000	0.011757000
P	-2.583788000	2.031471000	-1.172190000
P	2.156831000	-1.903265000	-1.746185000
P	3.013955000	2.238832000	0.154915000
P	-2.923222000	-0.418953000	2.570567000
N	3.657814000	-0.660711000	0.499202000
N	-3.371980000	-0.699484000	-0.346730000
N	0.002085000	-0.747824000	0.495060000
N	0.167079000	0.673748000	0.951109000
C	4.102107000	-1.978349000	0.236964000
C	-3.760678000	0.960045000	-2.097791000
C	-4.800760000	-2.715759000	-0.275691000
C	3.993419000	-4.017400000	-1.128077000
H	3.535023000	-4.582666000	-1.939093000
C	-4.522347000	-2.804688000	2.519043000
H	-4.402756000	-2.852520000	3.601451000
C	4.538988000	0.163679000	1.232705000
C	-4.010959000	-1.728595000	0.372883000
C	-3.962714000	-0.351004000	-1.574162000
C	2.356730000	3.661005000	1.203926000
H	3.164969000	4.401763000	1.310745000
C	-5.457464000	-0.832460000	-3.443774000
H	-6.099400000	-1.539515000	-3.972272000
C	-3.897648000	-1.771132000	1.796387000
C	3.533408000	-2.718925000	-0.843919000
C	4.410650000	1.584397000	1.158365000
C	5.029293000	-4.597391000	-0.386119000
C	5.614681000	-1.874505000	2.245186000
C	5.573017000	-0.376449000	2.045070000
C	5.119867000	-2.595581000	1.012050000
C	6.344486000	1.866125000	2.628915000
C	-3.684947000	2.084318000	3.725499000
H	-3.037927000	2.046570000	4.611687000
H	-4.513938000	2.771812000	3.950608000
H	-3.100239000	2.507609000	2.897586000
C	-1.310990000	2.628731000	-2.460245000
H	-0.490112000	3.010018000	-1.833993000
C	-5.445642000	-3.703072000	0.476685000
H	-6.051796000	-4.447555000	-0.042526000
C	-3.614319000	3.582836000	-0.804009000
H	-3.916098000	4.013356000	-1.771555000
C	6.468819000	0.472624000	2.703596000
H	7.259924000	0.028989000	3.310670000
C	-4.792750000	-1.256326000	-2.287814000
C	-1.964348000	-1.239127000	3.972990000
H	-2.697588000	-1.598757000	4.712449000
C	-5.303050000	-3.768569000	1.870444000
C	5.582207000	-3.873977000	0.678192000
H	6.372362000	-4.319007000	1.285550000
C	-0.773167000	1.419505000	-3.251335000
H	-0.379249000	0.644751000	-2.578414000
H	0.044219000	1.742458000	-3.913994000
H	-1.562044000	0.971811000	-3.870712000
C	4.102388000	-0.601826000	-3.295033000
H	3.884060000	0.269744000	-2.664859000
H	4.445047000	-0.243550000	-4.277225000
H	4.924573000	-1.159475000	-2.826465000
C	5.300784000	2.408698000	1.871341000
H	5.175211000	3.490531000	1.836712000
C	-4.859332000	-2.684265000	-1.788419000
C	3.874695000	3.014676000	-1.353698000
H	4.601045000	2.231108000	-1.619868000
C	-2.774414000	4.614031000	-0.027693000
H	-2.429026000	4.191317000	0.926785000
H	-3.378491000	5.506614000	0.194438000
H	-1.888600000	4.939209000	-0.589928000
C	-4.441297000	1.352589000	-3.265967000
H	-4.320293000	2.366749000	-3.644109000
C	0.911022000	-3.279053000	-2.058324000
H	1.420796000	-4.058653000	-2.646222000
C	1.958841000	3.144042000	2.602702000
H	1.191183000	2.363846000	2.517350000
H	1.550928000	3.977702000	3.194915000
H	2.819326000	2.730051000	3.142667000
C	-4.244450000	0.691359000	3.368878000
H	-4.951981000	0.813537000	2.533648000
C	-1.020387000	-0.222088000	4.649867000
H	-0.326091000	0.203964000	3.913379000
H	-0.430141000	-0.731078000	5.426573000
H	-1.564207000	0.600235000	5.131838000
C	-4.999680000	0.066303000	4.555509000
H	-5.455288000	-0.894761000	4.287000000
H	-5.807281000	0.741108000	4.877790000
H	-4.336537000	-0.087858000	5.418404000
C	-5.299436000	0.471257000	-3.935795000
C	-1.746675000	3.751699000	-3.422167000
H	-2.533609000	3.414229000	-4.109061000
H	-0.884883000	4.051827000	-4.038077000
H	-2.104624000	4.647527000	-2.899124000
C	0.434174000	-3.895124000	-0.727757000
H	1.267630000	-4.340981000	-0.169961000
H	-0.301505000	-4.687114000	-0.935347000
H	-0.039350000	-3.135002000	-0.094687000
C	1.149531000	4.331726000	0.520284000
H	1.408319000	4.773363000	-0.451335000
H	0.763541000	5.139086000	1.160810000
H	0.345743000	3.598977000	0.372518000
C	2.860210000	-1.498579000	-3.461591000
H	2.064215000	-0.903628000	-3.937409000
C	-0.278599000	-2.737764000	-2.877817000
H	-0.807249000	-1.955431000	-2.317784000
H	-0.990258000	-3.552669000	-3.078586000
H	0.033234000	-2.321229000	-3.846032000
C	4.653197000	4.313667000	-1.077301000
H	3.981024000	5.133896000	-0.788738000
H	5.182918000	4.627613000	-1.989460000
H	5.402391000	4.180673000	-0.287419000
C	-4.886478000	3.201572000	-0.025174000
H	-5.513836000	2.506301000	-0.596494000
H	-5.477558000	4.104260000	0.191841000
H	-4.631613000	2.725069000	0.931147000
C	-1.156505000	-2.441789000	3.441644000
H	-1.807478000	-3.215751000	3.016747000
H	-0.586517000	-2.887852000	4.270878000
H	-0.451245000	-2.120481000	2.663751000
C	3.179588000	-2.709880000	-4.356403000
H	3.955053000	-3.341214000	-3.902022000
H	3.563458000	-2.359438000	-5.326665000
H	2.296154000	-3.330462000	-4.555104000
C	2.902051000	3.181533000	-2.539206000
H	2.342978000	2.256002000	-2.729811000
H	3.463152000	3.443229000	-3.449002000
H	2.174939000	3.984341000	-2.356864000
H	7.036854000	2.515076000	3.163010000
H	6.627523000	-2.206894000	2.515997000
H	4.963829000	-2.139948000	3.101418000
H	5.387164000	-5.598375000	-0.622273000
H	-5.792389000	-4.557301000	2.439963000
H	-5.761933000	-3.191894000	-2.158325000
H	-3.996135000	-3.247024000	-2.194942000
H	-5.829628000	0.792221000	-4.831385000

TS_{K5m}(closed-shell singlet)

Ti	1.684365000	0.232694000	-0.466733000
Ti	-1.616308000	0.352082000	0.250358000
P	2.979423000	2.435193000	0.022019000
P	-2.346231000	-0.901683000	2.442909000
P	-3.197274000	2.213861000	-0.433372000
P	2.213665000	-1.812309000	-1.905844000
N	-3.188364000	-0.751790000	-0.360610000
N	3.611817000	-0.462738000	0.343737000
N	-0.130283000	0.697551000	-0.824773000
N	0.344573000	-0.096469000	0.663139000
C	-3.489575000	-2.020050000	0.177770000
C	4.442292000	1.789329000	0.888594000
C	4.933584000	-2.427340000	1.096967000
C	-3.394862000	-3.573523000	2.059305000
H	-3.094759000	-3.806803000	3.080565000
C	3.790245000	-3.976737000	-0.940839000
H	3.330591000	-4.583242000	-1.721353000
C	-4.028524000	-0.281564000	-1.389339000
C	3.982606000	-1.816066000	0.232637000
C	4.510869000	0.366042000	1.032569000
C	-2.561441000	3.580238000	-1.585628000
H	-3.447589000	4.098874000	-1.983375000
C	6.525775000	0.687360000	2.393403000
H	7.311620000	0.249424000	3.011680000
C	3.420985000	-2.624560000	-0.805806000
C	-3.121007000	-2.300724000	1.525069000
C	-4.170221000	1.126113000	-1.567795000
C	-4.066870000	-4.540962000	1.299381000
C	-4.499755000	-2.665962000	-2.032808000
C	-4.745176000	-1.179573000	-2.213838000
C	-4.170532000	-2.995350000	-0.588999000
C	-5.715213000	0.707959000	-3.417224000
C	2.512741000	-0.430552000	-4.400467000
H	1.605170000	-0.813897000	-4.883769000
H	3.205317000	-0.116199000	-5.195474000
H	2.228136000	0.461265000	-3.824531000
C	2.099879000	3.625785000	1.204074000
H	1.160663000	3.846677000	0.673927000
C	5.308625000	-3.762417000	0.914662000
H	6.043844000	-4.195001000	1.595590000
C	3.642990000	3.522710000	-1.367440000
H	4.263492000	4.299093000	-0.892937000
C	-5.594120000	-0.672294000	-3.208382000
H	-6.146717000	-1.369592000	-3.840068000
C	5.537594000	-0.153428000	1.876923000
C	0.910643000	-3.115664000	-2.287299000
H	1.426071000	-3.956511000	-2.778186000
C	4.739709000	-4.554170000	-0.092808000
C	-4.462971000	-4.238384000	-0.011541000
H	-4.991721000	-4.985964000	-0.605208000
C	1.748052000	2.877220000	2.505584000
H	1.197677000	1.951011000	2.294092000
H	1.122790000	3.518530000	3.144710000
H	2.658642000	2.620271000	3.064252000
C	-5.019921000	-0.097334000	2.817156000
H	-4.815793000	0.492091000	1.914559000
H	-5.760928000	0.439918000	3.427646000
H	-5.462015000	-1.051792000	2.501132000
C	-4.996570000	1.597981000	-2.606244000
H	-5.090776000	2.669469000	-2.779523000
C	5.465109000	-1.614229000	2.253404000
C	-4.549447000	3.107453000	0.604893000
H	-5.249684000	2.282659000	0.805650000
C	2.494216000	4.201343000	-2.139466000
H	1.828490000	3.454820000	-2.594585000
H	2.903643000	4.826864000	-2.946594000
H	1.883634000	4.845440000	-1.493062000
C	5.454167000	2.611702000	1.424839000
H	5.412717000	3.687273000	1.256951000
C	-1.095172000	-1.700650000	3.604397000
H	-1.652004000	-2.358935000	4.289507000
C	-1.762322000	2.995776000	-2.764971000
H	-0.899349000	2.423680000	-2.400144000
H	-1.402684000	3.816377000	-3.405871000
H	-2.379413000	2.326835000	-3.377498000
C	3.186170000	-1.496964000	-3.510920000
H	4.118229000	-1.064910000	-3.112655000
C	-0.167937000	-2.566425000	-3.244188000
H	-0.641269000	-1.668240000	-2.826380000
H	-0.947432000	-3.329440000	-3.389407000
H	0.238880000	-2.317784000	-4.232509000
C	3.545305000	-2.761964000	-4.310846000
H	4.077289000	-3.493870000	-3.690291000
H	4.201314000	-2.497176000	-5.153977000
H	2.649101000	-3.241885000	-4.728904000
C	6.516604000	2.070927000	2.152606000
C	2.816484000	4.955400000	1.506661000
H	3.730970000	4.790124000	2.090318000
H	2.153176000	5.594132000	2.109147000
H	3.077967000	5.515278000	0.598679000
C	-0.061252000	-2.548926000	2.839883000
H	-0.539869000	-3.375627000	2.299615000
H	0.656965000	-2.979765000	3.554881000
H	0.490507000	-1.936520000	2.115323000
C	-1.709132000	4.599472000	-0.803214000
H	-2.274232000	5.095364000	-0.003495000
H	-1.338587000	5.380567000	-1.484771000
H	-0.839583000	4.103636000	-0.351418000
C	-3.734513000	-0.339122000	3.630661000
H	-3.374240000	0.631906000	4.007476000
C	-0.401713000	-0.599675000	4.435433000
H	0.167675000	0.071915000	3.779873000
H	0.300626000	-1.056110000	5.149024000
H	-1.118018000	0.004158000	5.011071000
C	-5.336053000	4.231581000	-0.093548000
H	-4.697896000	5.096827000	-0.321577000
H	-6.142343000	4.586447000	0.567311000
H	-5.802214000	3.888403000	-1.025775000
C	4.543320000	2.694254000	-2.304629000
H	5.368252000	2.223662000	-1.755491000
H	4.970025000	3.344091000	-3.083183000
H	3.970195000	1.901512000	-2.805631000
C	0.273396000	-3.618036000	-0.976404000
H	1.018510000	-4.065449000	-0.307503000
H	-0.488253000	-4.377677000	-1.207008000
H	-0.212962000	-2.794283000	-0.439606000
C	-4.024181000	-1.261607000	4.828760000
H	-4.325719000	-2.263305000	4.491996000
H	-4.857165000	-0.848132000	5.418364000
H	-3.163508000	-1.364274000	5.502091000
C	-3.974631000	3.575378000	1.956394000
H	-3.402811000	2.771543000	2.440971000
H	-4.788961000	3.878868000	2.631663000
H	-3.305364000	4.439215000	1.836751000
H	-6.366848000	1.089077000	-4.202588000
H	-3.651047000	-2.971487000	-2.675085000
H	-5.367398000	-3.248424000	-2.376293000
H	-4.286586000	-5.518425000	1.726869000
H	4.784452000	-1.727153000	3.120283000
H	6.446094000	-1.988331000	2.581072000
H	7.301288000	2.711391000	2.552080000
H	5.027047000	-5.597987000	-0.209565000

TS_{K5m}(open-shell singlet)

Ti	1.656380000	0.287276000	-0.412467000
Ti	-1.589202000	0.401548000	0.307844000

P	3.039124000	2.406890000	0.067462000
P	-2.276842000	-1.037134000	2.426112000
P	-3.217128000	2.281997000	-0.352331000
P	2.099377000	-1.732314000	-1.948872000
N	-3.203092000	-0.702800000	-0.333336000
N	3.580950000	-0.521611000	0.301305000
N	-0.140153000	0.826287000	-0.789276000
N	0.330883000	0.114582000	0.813055000
C	-3.491086000	-2.003566000	0.135305000
C	4.489432000	1.685752000	0.904725000
C	4.868802000	-2.546199000	0.950665000
C	-3.365737000	-3.666032000	1.928176000
H	-3.044311000	-3.952119000	2.929474000
C	3.652422000	-3.981869000	-1.128869000
H	3.164581000	-4.544008000	-1.925502000
C	-4.045345000	-0.199433000	-1.345816000
C	3.917044000	-1.877765000	0.129987000
C	4.514472000	0.257642000	1.005901000
C	-2.597413000	3.681485000	-1.462417000
H	-3.485413000	4.220210000	-1.828515000
C	6.549222000	0.473381000	2.358687000
H	7.327566000	-0.008571000	2.953369000
C	3.312892000	-2.631554000	-0.925177000
C	-3.096684000	-2.368913000	1.456230000
C	-4.195219000	1.213419000	-1.494084000
C	-4.051615000	-4.593198000	1.131834000
C	-4.519678000	-2.555387000	-2.092186000
C	-4.770799000	-1.064997000	-2.203888000
C	-4.179506000	-2.946110000	-0.668287000
C	-5.763663000	0.856824000	-3.336076000
C	2.392759000	-0.181577000	-4.342916000
H	1.483647000	-0.530407000	-4.848846000
H	3.084386000	0.183800000	-5.116770000
H	2.111147000	0.670281000	-3.707778000
C	2.217496000	3.607665000	1.285016000
H	1.265205000	3.843873000	0.785213000
C	5.211276000	-3.879349000	0.702824000
H	5.949545000	-4.356704000	1.349851000
C	3.743270000	3.509607000	-1.292801000
H	4.376224000	4.265569000	-0.802180000
C	-5.631026000	-0.528420000	-3.170186000
H	-6.185615000	-1.209169000	-3.818289000
C	5.535789000	-0.321161000	1.816632000
C	0.788961000	-2.997977000	-2.416486000
H	1.295660000	-3.820793000	-2.945342000
C	4.608206000	-4.614367000	-0.327602000
C	-4.462650000	-4.218527000	-0.154941000
H	-4.996175000	-4.933308000	-0.783980000
C	1.894479000	2.868753000	2.599413000
H	1.315039000	1.956941000	2.406306000
H	1.307280000	3.527417000	3.257399000
H	2.817862000	2.593393000	3.127496000
C	-4.919934000	-0.189746000	2.901598000
H	-4.726222000	0.451069000	2.032594000
H	-5.636925000	0.320740000	3.561725000
H	-5.386977000	-1.113975000	2.536036000
C	-5.034631000	1.717516000	-2.505716000
H	-5.126874000	2.794627000	-2.643195000
C	5.433221000	-1.794738000	2.133109000
C	-4.537766000	3.094986000	0.766235000
H	-5.218359000	2.252314000	0.959018000
C	2.609446000	4.219481000	-2.058442000
H	1.932646000	3.487923000	-2.522162000
H	3.029910000	4.848929000	-2.856921000
H	2.007456000	4.864227000	-1.404159000
C	5.524194000	2.459253000	1.466994000
H	5.513896000	3.540523000	1.334489000
C	-1.001018000	-1.897508000	3.510563000
H	-1.539822000	-2.588505000	4.177710000
C	-1.817520000	3.129616000	-2.671668000
H	-0.953450000	2.541524000	-2.335677000
H	-1.460078000	3.969738000	-3.287488000
H	-2.447116000	2.487103000	-3.299394000
C	3.066784000	-1.306236000	-3.528383000
H	4.000266000	-0.903340000	-3.103945000
C	-0.274091000	-2.385103000	-3.351692000
H	-0.731110000	-1.496442000	-2.896539000
H	-1.068438000	-3.124611000	-3.533390000
H	0.142212000	-2.101852000	-4.326546000
C	3.421585000	-2.517602000	-4.408959000
H	3.951379000	-3.289516000	-3.836572000
H	4.077699000	-2.200997000	-5.233891000
H	2.523423000	-2.967190000	-4.855720000
C	6.573542000	1.864107000	2.172568000
C	2.963057000	4.926960000	1.563842000
H	3.897863000	4.748989000	2.110608000
H	2.331870000	5.570095000	2.195692000
H	3.195230000	5.489169000	0.649636000
C	0.010211000	-2.706964000	2.676858000
H	-0.483990000	-3.502148000	2.104384000
H	0.744269000	-3.176682000	3.349736000
H	0.545417000	-2.053763000	1.976357000
C	-1.722895000	4.662305000	-0.655031000
H	-2.272849000	5.138710000	0.167012000
H	-1.352068000	5.460690000	-1.315536000
H	-0.854429000	4.139604000	-0.232310000
C	-3.622272000	-0.506465000	3.669694000
H	-3.231089000	0.431854000	4.095206000
C	-0.281568000	-0.834605000	4.368599000
H	0.260722000	-0.131399000	3.723080000
H	0.446373000	-1.321831000	5.034405000
H	-0.979113000	-0.262569000	4.997349000
C	-5.360835000	4.228518000	0.127252000
H	-4.741676000	5.110344000	-0.088361000
H	-6.153111000	4.546389000	0.822163000
H	-5.846422000	3.907610000	-0.802955000
C	4.631226000	2.680564000	-2.240647000
H	5.452172000	2.195109000	-1.698445000
H	5.063322000	3.332582000	-3.014553000
H	4.046880000	1.899333000	-2.746538000
C	0.132446000	-3.555264000	-1.137745000
H	0.865921000	-4.037681000	-0.480334000
H	-0.633198000	-4.297239000	-1.408591000
H	-0.357516000	-2.752792000	-0.571376000
C	-3.907561000	-1.491129000	4.818242000
H	-4.238623000	-2.464430000	4.430132000
H	-4.717787000	-1.094668000	5.449530000
H	-3.034718000	-1.651167000	5.464008000
C	-3.926681000	3.527658000	2.114718000
H	-3.348540000	2.711465000	2.569294000
H	-4.724734000	3.818046000	2.814447000
H	-3.256597000	4.390790000	1.999825000
H	-6.424375000	1.260273000	-4.102145000
H	-3.672602000	-2.826183000	-2.751926000
H	-5.386098000	-3.125820000	-2.458105000
H	-4.264383000	-5.592519000	1.509067000
H	4.759880000	-1.928719000	3.002856000
H	6.408857000	-2.204631000	2.432876000
H	7.376648000	2.468577000	2.591275000
H	4.872096000	-5.657384000	-0.495632000

TS_{K5m}(triplet)

Ti	1.646443000	0.284168000	-0.365656000
Ti	-1.577522000	0.404338000	0.328837000
P	3.045970000	2.393766000	0.088136000
P	-2.294384000	-1.051513000	2.430506000
P	-3.207892000	2.296932000	-0.354263000
P	2.075407000	-1.718858000	-1.942717000

N	-3.199985000	-0.692499000	-0.337797000
N	3.586676000	-0.541452000	0.297973000
N	-0.127445000	0.842216000	-0.781898000
N	0.321710000	0.134655000	0.873035000
C	-3.498640000	-1.993665000	0.121556000
C	4.500464000	1.660678000	0.911609000
C	4.889707000	-2.570249000	0.900459000
C	-3.399256000	-3.666235000	1.907903000
H	-3.087668000	-3.958556000	2.910547000
C	3.648483000	-3.979043000	-1.183383000
H	3.150840000	-4.531307000	-1.980884000
C	-4.023858000	-0.183656000	-1.361039000
C	3.924249000	-1.893337000	0.102700000
C	4.527089000	0.231724000	0.999753000
C	-2.585029000	3.711652000	-1.440238000
H	-3.470277000	4.247393000	-1.817454000
C	6.575516000	0.434712000	2.333933000
H	7.360965000	-0.052843000	2.914571000
C	3.305984000	-2.634049000	-0.953319000
C	-3.117994000	-2.368597000	1.444288000
C	-4.163656000	1.230347000	-1.514704000
C	-4.083348000	-4.586258000	1.102065000
C	-4.505287000	-2.535256000	-2.118565000
C	-4.745089000	-1.043337000	-2.230870000
C	-4.184147000	-2.930660000	-0.691760000
C	-5.713436000	0.884953000	-3.374191000
C	2.333577000	-0.111472000	-4.302117000
H	1.422991000	-0.456736000	-4.807781000
H	3.015410000	0.276667000	-5.073622000
H	2.050521000	0.722969000	-3.645030000
C	2.238906000	3.591635000	1.319033000
H	1.280054000	3.826835000	0.831329000
C	5.234219000	-3.897587000	0.626564000
H	5.983704000	-4.381931000	1.255294000
C	3.751826000	3.503413000	-1.266239000
H	4.389227000	4.253888000	-0.772909000
C	-5.590638000	-0.501436000	-3.205679000
H	-6.142571000	-1.179034000	-3.859413000
C	5.558713000	-0.355251000	1.791455000
C	0.769938000	-2.983136000	-2.424981000
H	1.277873000	-3.796939000	-2.966393000
C	4.619654000	-4.619149000	-0.406758000
C	-4.479481000	-4.203505000	-0.186988000
H	-5.010188000	-4.912610000	-0.824835000
C	1.933198000	2.851853000	2.637190000
H	1.351897000	1.939878000	2.450979000
H	1.353982000	3.510163000	3.302711000
H	2.863394000	2.577284000	3.153567000
C	-4.937384000	-0.205128000	2.910090000
H	-4.743752000	0.438959000	2.043539000
H	-5.653964000	0.303424000	3.572191000
H	-5.405338000	-1.127237000	2.540482000
C	-4.987760000	1.739882000	-2.536178000
H	-5.070418000	2.817739000	-2.674535000
C	5.464349000	-1.833843000	2.087653000
C	-4.541353000	3.076630000	0.765637000
H	-5.212272000	2.223542000	0.945611000
C	2.618107000	4.221281000	-2.024294000
H	1.936946000	3.493813000	-2.487896000
H	3.037813000	4.852797000	-2.821586000
H	2.020997000	4.865294000	-1.364718000
C	5.538263000	2.428903000	1.475178000
H	5.526097000	3.511483000	1.354167000
C	-1.025842000	-1.930172000	3.509351000
H	-1.570064000	-2.621404000	4.171768000
C	-1.779341000	3.173969000	-2.639395000
H	-0.919181000	2.586455000	-2.292065000
H	-1.413921000	4.021228000	-3.240417000
H	-2.393782000	2.534508000	-3.285014000
C	3.024302000	-1.248433000	-3.519140000
H	3.958374000	-0.847579000	-3.094199000
C	-0.298906000	-2.362560000	-3.348289000
H	-0.756178000	-1.480145000	-2.881402000
H	-1.091926000	-3.102251000	-3.534842000
H	0.112403000	-2.067424000	-4.321715000
C	3.380525000	-2.438009000	-4.428492000
H	3.921248000	-3.217770000	-3.877249000
H	4.026718000	-2.098564000	-5.252135000
H	2.481878000	-2.885117000	-4.876752000
C	6.594202000	1.827616000	2.165861000
C	2.985031000	4.912289000	1.590363000
H	3.926882000	4.736062000	2.125516000
H	2.360121000	5.552965000	2.230956000
H	3.204745000	5.476474000	0.674386000
C	-0.019690000	-2.742379000	2.672268000
H	-0.519287000	-3.527837000	2.091155000
H	0.707646000	-3.224551000	3.343614000
H	0.524011000	-2.087956000	1.979710000
C	-1.732172000	4.691696000	-0.608867000
H	-2.301943000	5.160926000	0.203816000
H	-1.351920000	5.495578000	-1.257047000
H	-0.869817000	4.171386000	-0.170789000
C	-3.640149000	-0.527121000	3.677037000
H	-3.248789000	0.408349000	4.108715000
C	-0.299185000	-0.876956000	4.373157000
H	0.246437000	-0.173467000	3.730543000
H	0.426484000	-1.372109000	5.035578000
H	-0.992843000	-0.304374000	5.005762000
C	-5.374271000	4.204773000	0.129994000
H	-4.764941000	5.096149000	-0.073934000
H	-6.175858000	4.506072000	0.821379000
H	-5.847906000	3.884308000	-0.806546000
C	4.633389000	2.676636000	-2.221866000
H	5.456237000	2.187544000	-1.685824000
H	5.062795000	3.330902000	-2.995393000
H	4.044654000	1.898748000	-2.727625000
C	0.120323000	-3.559680000	-1.151070000
H	0.858526000	-4.045423000	-0.501297000
H	-0.641572000	-4.303173000	-1.428161000
H	-0.373777000	-2.767040000	-0.574200000
C	-3.928146000	-1.517053000	4.820396000
H	-4.261088000	-2.487687000	4.427321000
H	-4.737855000	-1.122101000	5.453333000
H	-3.055960000	-1.682167000	5.465738000
C	-3.944298000	3.503955000	2.122432000
H	-3.365321000	2.688608000	2.577334000
H	-4.750596000	3.783646000	2.816957000
H	-3.279385000	4.372373000	2.019675000
H	-6.362659000	1.292161000	-4.147962000
H	-3.652059000	-2.809906000	-2.768567000
H	-5.370779000	-3.099419000	-2.496199000
H	-4.305326000	-5.585896000	1.473082000
H	4.800403000	-1.982906000	2.962204000
H	6.444420000	-2.244527000	2.371436000
H	7.399509000	2.428873000	2.585010000
H	4.885585000	-5.658226000	-0.594719000

5m(closed-shell singlet)

Ti	-1.484520000	-0.024465000	-0.083007000
Ti	1.128413000	0.347535000	-0.034124000
P	-1.978031000	-2.551170000	-0.307133000
P	2.582851000	2.180726000	-1.371015000
P	-2.411966000	2.215410000	0.799987000
P	2.967210000	-0.233895000	2.243142000
N	-3.794615000	-0.184831000	-0.338493000
N	2.727757000	-0.759725000	-0.687833000
N	-0.203497000	0.483203000	-1.270678000
N	-0.176327000	-0.156722000	1.165721000

C	-4.405601000	-1.338296000	-0.870418000
C	3.813701000	-2.965768000	-0.723706000
C	3.296756000	-1.857362000	-0.005919000
C	-4.674772000	0.813205000	0.106822000
C	3.386249000	-1.833049000	1.415187000
C	3.236351000	-0.492688000	-1.974782000
C	3.242919000	0.845570000	-2.471549000
C	1.908361000	3.451931000	-2.591294000
H	2.745404000	3.723737000	-3.253662000
C	-3.677972000	-2.567351000	-0.956321000
C	-6.076767000	0.803525000	-0.177402000
C	-5.763625000	-1.371631000	-1.310389000
C	-4.272116000	-3.731371000	-1.479118000
H	-3.686243000	-4.647698000	-1.544713000
C	-4.200296000	1.916148000	0.887152000
C	-1.011238000	-3.716202000	-1.414566000
H	-1.598966000	-4.642040000	-1.512161000
C	3.788397000	-1.532295000	-2.767274000
C	-2.252845000	3.669634000	-0.397520000
H	-1.166401000	3.774551000	-0.532405000
C	3.761643000	1.095789000	-3.756775000
H	3.750003000	2.108379000	-4.158052000
C	4.336035000	-1.238619000	-4.019782000
H	4.761418000	-2.048120000	-4.615049000
C	-2.067865000	-3.398940000	1.377829000
H	-1.027819000	-3.382194000	1.737063000
C	-5.602972000	-3.739637000	-1.902781000
C	4.369029000	-4.044524000	-0.025749000
H	4.763690000	-4.892323000	-0.588148000
C	3.690330000	-2.947476000	-2.234534000
C	-6.946522000	1.673733000	0.483887000
H	-8.014638000	1.600254000	0.269762000
C	4.317447000	0.068150000	-4.527397000
C	-6.559962000	-0.090916000	-1.290486000
C	3.915856000	-2.951996000	2.085162000
H	3.968068000	-2.951417000	3.173734000
C	-1.887204000	2.878716000	2.474440000
H	-2.527458000	3.746292000	2.699145000
C	0.775768000	2.849722000	-3.446523000
H	1.135501000	2.012493000	-4.056190000
H	0.380266000	3.624840000	-4.120870000
H	-0.035595000	2.466773000	-2.817749000
C	-6.335718000	-2.550802000	-1.796092000
H	-7.379154000	-2.525184000	-2.116151000
C	4.402576000	-4.057998000	1.376016000
C	1.448820000	4.737516000	-1.873211000
H	0.692620000	4.521989000	-1.107598000
H	0.998281000	5.423729000	-2.605332000
H	2.280283000	5.266357000	-1.390797000
C	-5.097324000	2.795957000	1.523303000
H	-4.703534000	3.601200000	2.143793000
C	2.265337000	-0.745391000	3.921917000
H	3.067119000	-1.249283000	4.483077000
C	4.723200000	0.406947000	2.701800000
H	4.582235000	1.493426000	2.812412000
C	5.340340000	-0.134248000	4.005405000
H	4.749940000	0.118826000	4.894839000
H	6.343218000	0.300246000	4.140022000
H	5.460489000	-1.225991000	3.965731000
C	4.157484000	2.962199000	-0.654375000
H	4.732819000	2.073817000	-0.360998000
C	-6.479415000	2.651025000	1.376142000
C	0.350581000	-4.066539000	-0.788627000
H	0.949498000	-3.164641000	-0.614735000
H	0.912015000	-4.722555000	-1.470383000
H	0.246447000	-4.595182000	0.167914000
C	-2.576685000	-4.850833000	1.334324000
H	-3.611978000	-4.892515000	0.970255000
H	-2.559213000	-5.278318000	2.348318000
H	-1.958539000	-5.493355000	0.692288000
C	1.854177000	0.527652000	4.691850000
H	2.686946000	1.236835000	4.806196000
H	1.500409000	0.261851000	5.699333000
H	1.037677000	1.041797000	4.169402000
C	-2.918835000	-2.536477000	2.332552000
H	-2.502699000	-1.525360000	2.431090000
H	-2.938289000	-2.998128000	3.331370000
H	-3.953986000	-2.453369000	1.974452000
C	1.075279000	-1.715669000	3.791119000
H	0.287684000	-1.277851000	3.165878000
H	0.670541000	-1.931844000	4.792613000
H	1.383524000	-2.666121000	3.336227000
C	-0.852869000	-3.078949000	-2.810403000
H	-1.829251000	-2.876757000	-3.270109000
H	-0.299354000	-3.763057000	-3.471431000
H	-0.302134000	-2.130816000	-2.746759000
C	-2.110376000	1.798630000	3.551305000
H	-3.163903000	1.493187000	3.598433000
H	-1.821291000	2.189837000	4.538523000
H	-1.498536000	0.913895000	3.331378000
C	-2.834343000	5.003737000	0.102408000
H	-3.918200000	4.924123000	0.259505000
H	-2.663055000	5.785699000	-0.653039000
H	-2.371029000	5.340583000	1.039828000
C	-2.866319000	3.267493000	-1.754325000
H	-2.434784000	2.329478000	-2.127467000
H	-2.674787000	4.056077000	-2.497190000
H	-3.953204000	3.137652000	-1.665459000
C	-0.417811000	3.341606000	2.437115000
H	0.238641000	2.502250000	2.166358000
H	-0.114010000	3.704474000	3.430507000
H	-0.256349000	4.157501000	1.718994000
C	5.703686000	0.159859000	1.535592000
H	5.996474000	-0.897390000	1.498371000
H	6.613477000	0.762750000	1.675998000
H	5.270280000	0.410823000	0.559947000
C	3.857146000	3.763017000	0.630549000
H	3.305153000	4.688478000	0.419955000
H	4.799964000	4.045791000	1.122380000
H	3.264413000	3.169092000	1.339136000
C	5.009538000	3.764072000	-1.654543000
H	5.254754000	3.168172000	-2.543159000
H	5.956354000	4.061656000	-1.179275000
H	4.502696000	4.683264000	-1.979676000
H	-7.171027000	3.310897000	1.897271000
H	-7.636272000	-0.298241000	-1.196304000
H	-6.432265000	0.438180000	-2.256326000
H	-6.057010000	-4.644449000	-2.303627000
H	2.707477000	-3.365166000	-2.522075000
H	4.449442000	-3.594318000	-2.697316000
H	4.733597000	0.283883000	-5.510313000
H	4.816988000	-4.913327000	1.908064000

TS$_{[2m-1]}$(closed-shell singlet)

Ti	1.401798000	0.359758000	-0.612686000
Ti	-1.419150000	0.366244000	0.147447000
P	2.689425000	2.554229000	-0.048960000
P	-1.650078000	-0.962382000	2.398221000
P	-3.316089000	2.123441000	-0.191826000
P	1.857825000	-1.844913000	-1.863219000
N	-3.010706000	-0.823439000	-0.223254000
N	3.340402000	-0.384133000	0.217618000
N	-0.411774000	0.902299000	-1.276944000
N	0.621721000	1.119159000	-2.086569000
C	-3.078410000	-2.127504000	0.299360000
C	4.273249000	1.881422000	0.546114000
C	4.688336000	-2.319015000	1.032353000
C	-2.469631000	-3.710090000	2.059012000

H	-1.955308000	-3.937851000	2.992066000
C	3.432944000	-3.988848000	-0.830500000
H	2.944947000	-4.631890000	-1.563077000
C	-4.012724000	-0.427981000	-1.122375000
C	3.694113000	-1.755609000	0.183501000
C	4.318154000	0.469152000	0.768759000
C	-3.010143000	3.623490000	-1.304309000
H	-3.997704000	4.061419000	-1.516793000
C	6.476256000	0.815179000	1.890219000
H	7.305406000	0.392422000	2.460646000
C	3.073196000	-2.631447000	-0.757982000
C	-2.419432000	-2.404312000	1.535248000
C	-4.278406000	0.964707000	-1.269588000
C	-3.189335000	-4.719948000	1.407177000
C	-4.415286000	-2.844279000	-1.716404000
C	-4.771629000	-1.375359000	-1.851684000
C	-3.793343000	-3.153400000	-0.366889000
C	-6.003839000	0.440980000	-2.918491000
C	2.114539000	3.755672000	1.305262000
H	1.048823000	3.908751000	1.073919000
C	5.040155000	-3.669325000	0.927280000
H	5.810121000	-4.058674000	1.595811000
C	3.111322000	3.633710000	-1.531455000
H	3.831335000	4.389947000	-1.179168000
C	-5.768095000	-0.928135000	-2.728057000
H	-6.349665000	-1.662250000	-3.288146000
C	5.407388000	-0.019190000	1.553156000
C	0.622209000	-3.169228000	-2.368777000
H	1.163563000	-3.907792000	-2.981541000
C	4.417116000	-4.522063000	0.008045000
C	-3.856116000	-4.429145000	0.207425000
H	-4.422139000	-5.211023000	-0.301844000
C	-5.253577000	1.378457000	-2.196535000
H	-5.439758000	2.440712000	-2.350694000
C	5.313699000	-1.430258000	2.077833000
C	-4.681353000	2.728891000	1.021764000
H	-5.233411000	1.797314000	1.215831000
C	5.363486000	2.699685000	0.901647000
H	5.327550000	3.762927000	0.666673000
C	-0.229880000	-1.698935000	3.406546000
H	-0.665834000	-2.433401000	4.100407000
C	2.921355000	-1.441907000	-3.391869000
H	3.672145000	-0.769795000	-2.944819000
C	6.491385000	2.172367000	1.536244000
C	-2.938131000	-0.567450000	3.767227000
H	-2.648210000	0.435455000	4.120685000
H	-0.587858000	2.768392000	3.109534000
H	-1.186060000	2.664002000	2.685004000
H	-6.768869000	0.774336000	-3.618359000
H	-5.301228000	-3.474272000	-1.886540000
H	-3.235139000	-5.721901000	1.831755000
H	-3.694851000	-3.111748000	-2.512464000
H	4.692888000	-5.573581000	-0.054599000
H	6.300525000	-1.808912000	2.381192000
H	4.684668000	-1.433838000	2.990332000
H	7.340271000	2.806615000	1.786208000
C	2.219550000	3.050020000	2.671822000
H	3.270424000	2.907084000	2.954851000
H	1.733396000	3.659761000	3.448092000
H	1.736912000	2.064090000	2.654362000
C	2.803524000	5.133412000	1.352154000
H	2.318151000	5.753265000	2.121470000
H	3.862099000	5.041296000	1.626648000
H	2.736118000	5.674162000	0.399904000
C	1.852443000	4.331238000	-2.080983000
H	1.375657000	4.982115000	-1.334853000
H	2.121940000	4.955483000	-2.946196000
H	1.122535000	3.579246000	-2.408247000
C	3.786574000	2.777438000	-2.621206000
H	4.684923000	2.273964000	-2.240544000
H	3.087636000	2.020287000	-2.999204000
H	4.082608000	3.418937000	-3.464926000
C	2.167110000	-0.657791000	-4.485834000
H	2.897454000	-0.177175000	-5.154201000
H	1.558347000	-1.331653000	-5.104357000
H	1.514873000	0.115799000	-4.060727000
C	3.657616000	-2.657885000	-3.984711000
H	4.331892000	-2.320494000	-4.786355000
H	4.259184000	-3.182791000	-3.233151000
H	2.951811000	-3.373470000	-4.431428000
C	-0.514784000	-2.551969000	-3.212247000
H	-0.155758000	-2.115033000	-4.150071000
H	-1.244381000	-3.336815000	-3.462966000
H	-1.034065000	-1.765200000	-2.648825000
C	0.037978000	-3.872687000	-1.127836000
H	0.808296000	-4.374364000	-0.531188000
H	-0.476886000	-3.151142000	-0.480950000
H	-0.699503000	-4.624351000	-1.445381000
C	-2.165680000	4.673141000	-0.552459000
H	-1.998663000	5.548798000	-1.197459000
H	-2.652505000	5.023633000	0.367522000
H	-1.184053000	4.258144000	-0.285665000
C	-2.349205000	3.243396000	-2.643087000
H	-2.220929000	4.154406000	-3.248444000
H	-1.368162000	2.781186000	-2.491392000
H	-2.966810000	2.538768000	-3.212953000
C	-5.681262000	3.755678000	0.458795000
H	-6.153616000	3.407388000	-0.467930000
H	-6.482753000	3.925757000	1.194126000
H	-5.204244000	4.726713000	0.265883000
C	-4.088179000	3.211940000	2.358447000
H	-3.503302000	4.134385000	2.237813000
H	-4.897721000	3.424255000	3.073271000
H	-3.433916000	2.451339000	2.801659000
C	0.439082000	-0.578513000	4.227831000
H	-0.266921000	-0.061554000	4.893137000
H	1.244432000	-0.996357000	4.849761000
H	0.885800000	0.166617000	3.555343000
C	0.802010000	-2.407801000	2.515601000
H	1.196469000	-1.716136000	1.757336000
H	1.643149000	-2.764290000	3.129678000
H	0.367823000	-3.270025000	1.995314000
C	-4.335539000	-0.475524000	3.124976000
H	-4.312849000	0.104892000	2.194543000
H	-4.712773000	-1.477793000	2.881680000
H	-5.044246000	-0.000967000	3.820007000
C	-2.974142000	-1.526797000	4.971110000
H	-3.782128000	-1.225630000	5.656036000
H	-3.184966000	-2.556091000	4.648097000
H	-2.038991000	-1.526140000	5.545149000

TS$_{[2m-1]}$(opem-shell singlet)

Ti	1.426600000	0.381919000	-0.612995000
Ti	-1.410269000	0.389336000	0.174384000
P	2.763067000	2.517426000	0.042819000
P	-1.627030000	-1.015072000	2.391691000
P	-3.252419000	2.186717000	-0.211868000
P	1.764513000	-1.796883000	-1.926306000
N	-3.054684000	-0.792460000	-0.162722000
N	3.331451000	-0.456891000	0.181180000
N	-0.393012000	0.922809000	-1.260977000
N	0.624427000	1.174552000	-2.067430000
C	-3.205201000	-2.085805000	0.377830000
C	4.325517000	1.767568000	0.607236000
C	4.619090000	-2.465443000	0.911381000
C	-2.709303000	-3.681784000	2.167115000
H	-2.206939000	-3.925566000	3.103005000
C	3.267778000	-4.029392000	-0.975647000

H	2.741543000	-4.631605000	-1.716406000
C	-4.034661000	-0.365144000	-1.077648000
C	3.634974000	-1.838664000	0.096405000
C	4.335714000	0.344903000	0.761934000
C	-2.934311000	3.675545000	-1.332750000
H	-3.915867000	4.131513000	-1.536275000
C	6.512009000	0.581867000	1.877373000
H	7.334622000	0.110855000	2.418771000
C	2.965130000	-2.661135000	-0.860768000
C	-2.565568000	-2.396888000	1.614278000
C	-4.246726000	1.034825000	-1.260367000
C	-3.496342000	-4.653392000	1.534244000
C	-4.551835000	-2.767029000	-1.640152000
C	-4.837085000	-1.286918000	-1.798142000
C	-3.979607000	-3.079712000	-0.271969000
C	-5.996249000	0.557810000	-2.899328000
C	2.249199000	3.726645000	1.416536000
H	1.184475000	3.909206000	1.203302000
C	4.914618000	-3.825365000	0.762106000
H	5.678936000	-4.264031000	1.406197000
C	3.224585000	3.602832000	-1.425813000
H	3.970819000	4.328938000	-1.065015000
C	-5.814209000	-0.815011000	-2.682076000
H	-6.425076000	-1.536828000	-3.226889000
C	5.418821000	-0.207652000	1.511511000
C	0.480588000	-3.064238000	-2.461033000
H	0.993942000	-3.810495000	-3.088297000
C	4.242426000	-4.625881000	-0.169014000
C	-4.129474000	-4.338705000	0.323636000
H	-4.735967000	-5.091625000	-0.182875000
C	-5.205114000	1.472363000	-2.193934000
H	-5.344850000	2.539309000	-2.364657000
C	5.295148000	-1.637624000	1.975360000
C	-4.564237000	2.805613000	1.039893000
H	-5.100185000	1.874278000	1.276263000
C	5.440356000	2.538651000	0.990803000
H	5.430174000	3.612489000	0.807581000
C	-0.185373000	-1.840892000	3.286647000
H	-0.607941000	-2.534192000	4.029592000
C	2.831474000	-1.404623000	-3.458461000
H	3.619128000	-0.783032000	-3.001488000
C	6.559570000	1.953459000	1.588697000
C	-2.764350000	-0.482359000	3.836870000
H	-2.374932000	0.504965000	4.132759000
H	-0.579511000	2.211729000	2.436680000
H	-0.786917000	2.835352000	2.784279000
H	-6.747106000	0.910015000	-3.605113000
H	-5.459778000	-3.359363000	-1.827694000
H	-3.610691000	-5.642596000	1.975265000
H	-3.821145000	-3.075528000	-2.412151000
H	4.473751000	-5.685565000	-0.265385000
H	6.277517000	-2.056704000	2.237703000
H	4.689655000	-1.662989000	2.903491000
H	7.426436000	2.553358000	1.860825000
C	2.356648000	3.017687000	2.781096000
H	3.408204000	2.860012000	3.053367000
H	1.884471000	3.633175000	3.561144000
H	1.858603000	2.040141000	2.769446000
C	2.973281000	5.087082000	1.456395000
H	2.516459000	5.714482000	2.237064000
H	4.034039000	4.969683000	1.712177000
H	2.902594000	5.634618000	0.508391000
C	1.990584000	4.349822000	-1.967073000
H	1.534091000	5.005283000	-1.212322000
H	2.281613000	4.977220000	-2.823054000
H	1.235991000	3.627749000	-2.306089000
C	3.869151000	2.737296000	-2.526825000
H	4.748617000	2.196813000	-2.153081000
H	3.144179000	2.010694000	-2.916452000
H	4.187981000	3.378112000	-3.362726000
C	2.107426000	-0.553816000	-4.522793000
H	2.854688000	-0.083581000	-5.179893000
H	1.467435000	-1.180505000	-5.159142000
H	1.489949000	0.232346000	-4.069885000
C	3.503013000	-2.635949000	-4.094933000
H	4.184566000	-2.307438000	-4.894243000
H	4.086677000	-3.210903000	-3.366219000
H	2.759513000	-3.303716000	-4.554349000
C	-0.632689000	-2.387553000	-3.290534000
H	-0.258826000	-1.946249000	-4.220562000
H	-1.392416000	-3.138619000	-3.555330000
H	-1.120591000	-1.593586000	-2.709391000
C	-0.132981000	-3.768715000	-1.235958000
H	0.617836000	-4.301535000	-0.641361000
H	-0.630631000	-3.039674000	-0.583580000
H	-0.890685000	-4.493303000	-1.569092000
C	-2.059308000	4.714053000	-0.599909000
H	-1.877716000	5.576413000	-1.258569000
H	-2.531020000	5.088971000	0.318056000
H	-1.085561000	4.280070000	-0.335642000
C	-2.294065000	3.273354000	-2.675893000
H	-2.159007000	4.177593000	-3.289711000
H	-1.317492000	2.799239000	-2.530918000
H	-2.927631000	2.573621000	-3.233926000
C	-5.592655000	3.810427000	0.489195000
H	-6.092142000	3.435217000	-0.412625000
H	-6.369631000	3.991020000	1.247681000
H	-5.130610000	4.780174000	0.257322000
C	-3.920842000	3.323723000	2.341170000
H	-3.365837000	4.257818000	2.178087000
H	-4.702548000	3.529454000	3.087986000
H	-3.227185000	2.587532000	2.764673000
C	0.641438000	-0.765712000	4.019952000
H	0.042258000	-0.185007000	4.735536000
H	1.465247000	-1.238545000	4.574826000
H	1.080308000	-0.068226000	3.293095000
C	0.698583000	-2.635474000	2.312317000
H	1.068771000	-1.984887000	1.506439000
H	1.570123000	-3.045162000	2.844424000
H	0.151230000	-3.468292000	1.855329000
C	-4.200544000	-0.305984000	3.307049000
H	-4.217505000	0.259873000	2.367952000
H	-4.661039000	-1.283883000	3.113755000
H	-4.816172000	0.224597000	4.048571000
C	-2.768151000	-1.404158000	5.070500000
H	-3.483655000	-1.017876000	5.812871000
H	-3.090030000	-2.420205000	4.802513000
H	-1.787610000	-1.466165000	5.558966000

$TS_{[2m-1]}$(triplet)

Ti	1.429231000	0.392550000	-0.646864000
Ti	-1.416095000	0.430399000	0.192211000
P	2.731308000	2.536929000	0.026193000
P	-1.514370000	-0.963722000	2.407999000
P	-3.356269000	2.140364000	-0.256756000
P	1.752533000	-1.791093000	-1.944242000
N	-3.034373000	-0.830229000	-0.103954000
N	3.333775000	-0.433804000	0.155742000
N	-0.380558000	0.970947000	-1.247612000
N	0.618320000	1.200962000	-2.083414000
C	-3.158811000	-2.103793000	0.490752000
C	4.292254000	1.799852000	0.615435000
C	4.642293000	-2.434467000	0.869591000
C	-2.635941000	-3.617030000	2.346013000
H	-2.121131000	-3.814157000	3.286228000
C	3.289496000	-4.004446000	-1.010468000
H	2.759592000	-4.609771000	-1.746014000
C	-4.035767000	-0.465596000	-1.025778000

C	3.648809000	-1.812189000	0.062206000
C	4.323561000	0.375200000	0.751971000
C	-3.079380000	3.606746000	-1.416035000
H	-4.070101000	4.038288000	-1.628254000
C	6.489256000	0.630655000	1.884471000
H	7.316100000	0.164414000	2.423590000
C	2.976844000	-2.638703000	-0.891046000
C	-2.501635000	-2.360019000	1.730264000
C	-4.298934000	0.918150000	-1.263810000
C	-3.425216000	-4.620953000	1.769629000
C	-4.495023000	-2.899667000	-1.489307000
C	-4.817095000	-1.436147000	-1.707274000
C	-3.925996000	-3.136882000	-0.106085000
C	-6.038650000	0.326160000	-2.875658000
C	2.202318000	3.784513000	1.360188000
H	1.144985000	3.969355000	1.114750000
C	4.948473000	-3.791306000	0.713765000
H	5.720326000	-4.225437000	1.351968000
C	3.212572000	3.595971000	-1.457317000
H	3.959558000	4.323878000	-1.101694000
C	-5.811816000	-1.030026000	-2.603374000
H	-6.402316000	-1.792647000	-3.114037000
C	5.411738000	-0.170926000	1.498498000
C	0.470102000	-3.071188000	-2.453315000
H	0.978384000	-3.816350000	-3.085898000
C	4.276347000	-4.594979000	-0.214533000
C	-4.064028000	-4.367696000	0.548067000
H	-4.664285000	-5.148396000	0.077429000
C	-5.274815000	1.289856000	-2.208134000
H	-5.447937000	2.345162000	-2.417088000
C	5.313113000	-1.609935000	1.939480000
C	-4.680357000	2.736158000	0.987694000
H	-5.156403000	1.786133000	1.273960000
C	5.392409000	2.582053000	1.018258000
H	5.368000000	3.657537000	0.847776000
C	-0.035058000	-1.773957000	3.252612000
H	-0.427165000	-2.408316000	4.061944000
C	2.793802000	-1.408354000	-3.498243000
H	3.590497000	-0.785696000	-3.058535000
C	6.515965000	2.006877000	1.617648000
C	-2.566258000	-0.356370000	3.887780000
H	-2.164377000	0.645898000	4.106950000
H	-0.631938000	2.333556000	2.259565000
H	-0.923714000	2.987361000	2.461961000
H	-6.801352000	0.626524000	-3.592512000
H	-5.385336000	-3.523088000	-1.659161000
H	-3.532276000	-5.588018000	2.258883000
H	-3.748886000	-3.219581000	-2.241735000
H	4.515482000	-5.652498000	-0.315521000
H	6.303873000	-2.017283000	2.188814000
H	4.715468000	-1.659665000	2.871815000
H	7.370602000	2.616955000	1.905455000
C	2.267618000	3.113347000	2.745692000
H	3.309899000	2.941584000	3.044412000
H	1.793589000	3.760830000	3.498440000
H	1.749098000	2.146768000	2.751964000
C	2.932671000	5.142362000	1.384973000
H	2.451209000	5.794763000	2.129615000
H	3.982751000	5.029026000	1.682750000
H	2.899218000	5.661900000	0.419467000
C	1.987767000	4.339461000	-2.023957000
H	1.529917000	5.014154000	-1.286998000
H	2.289383000	4.946427000	-2.891019000
H	1.231058000	3.614718000	-2.353107000
C	3.863824000	2.708841000	-2.536847000
H	4.733327000	2.165986000	-2.143579000
H	3.137452000	1.983376000	-2.926222000
H	4.199657000	3.333974000	-3.377994000
C	2.052848000	-0.561051000	-4.553798000
H	2.789114000	-0.095840000	-5.226734000
H	1.399777000	-1.189096000	-5.175329000
H	1.445629000	0.229290000	-4.094316000
C	3.453679000	-2.642239000	-4.141893000
H	4.120784000	-2.317207000	-4.954755000
H	4.050686000	-3.214122000	-3.421611000
H	2.702127000	-3.311921000	-4.585097000
C	-0.658825000	-2.402462000	-3.267830000
H	-0.300843000	-1.959514000	-4.203311000
H	-1.418024000	-3.157867000	-3.521545000
H	-1.142945000	-1.611356000	-2.679570000
C	-0.122453000	-3.774685000	-1.217564000
H	0.639606000	-4.299855000	-0.630332000
H	-0.617595000	-3.046012000	-0.562749000
H	-0.878057000	-4.506955000	-1.538912000
C	-2.218264000	4.679545000	-0.716328000
H	-2.052952000	5.525250000	-1.400244000
H	-2.692121000	5.073607000	0.192388000
H	-1.236786000	4.267674000	-0.444756000
C	-2.433228000	3.178503000	-2.748798000
H	-2.306638000	4.068688000	-3.384317000
H	-1.451297000	2.719953000	-2.588813000
H	-3.057877000	2.458363000	-3.290602000
C	-5.771742000	3.652675000	0.405543000
H	-6.256907000	3.206800000	-0.471437000
H	-6.549862000	3.823084000	1.165048000
H	-5.368916000	4.635431000	0.123455000
C	-4.054244000	3.352012000	2.254938000
H	-3.561831000	4.310649000	2.042015000
H	-4.839029000	3.543017000	3.002280000
H	-3.312103000	2.680753000	2.703496000
C	0.863743000	-0.681215000	3.864215000
H	0.322353000	-0.029982000	4.565202000
H	1.700242000	-1.143004000	4.409458000
H	1.285762000	-0.054326000	3.066544000
C	0.765700000	-2.654679000	2.280038000
H	1.118794000	-2.067675000	1.420740000
H	1.648582000	-3.067092000	2.790848000
H	0.165308000	-3.489840000	1.900875000
C	-4.030720000	-0.209273000	3.430287000
H	-4.102295000	0.304371000	2.463661000
H	-4.497782000	-1.196368000	3.315907000
H	-4.606121000	0.361280000	4.174426000
C	-2.497402000	-1.207869000	5.168961000
H	-3.169308000	-0.779602000	5.928812000
H	-2.832130000	-2.237095000	4.978142000
H	-1.489978000	-1.243340000	5.602448000

$TS_{[2m-2]}$(closed-shell singlet)

Ti	1.377248000	-0.207129000	-0.795486000
Ti	-1.327874000	0.400791000	-0.176333000
P	2.871611000	1.830048000	-1.383366000
P	-1.254092000	1.753231000	2.048971000
P	-3.359283000	0.675513000	-1.812105000
P	1.536269000	-2.755180000	-0.737255000
N	-2.927568000	-0.446418000	0.862460000
N	3.180129000	-0.473796000	0.431473000
N	-0.260869000	0.439380000	-1.727015000
N	0.723315000	0.145102000	-2.550749000
C	-2.974150000	-0.453279000	2.273320000
C	4.105023000	1.773597000	-0.047203000
C	4.334557000	-1.863821000	2.147252000
C	-2.402032000	0.596789000	4.407659000
H	-1.870120000	1.362852000	4.970032000
C	3.108003000	-4.164294000	1.145982000
H	2.590285000	-5.053360000	0.787617000
C	-4.003664000	-1.091536000	0.209025000
C	3.438986000	-1.719502000	1.046201000
C	4.068555000	0.581427000	0.751193000

C	-3.215354000	0.223933000	-3.638745000
H	-4.240616000	0.177159000	-4.039488000
C	5.914879000	1.535662000	2.062205000
H	6.600827000	1.434767000	2.905464000
C	2.804902000	-2.914044000	0.572929000
C	-2.295537000	0.563720000	3.004255000
C	-4.374972000	-0.682509000	-1.105412000
C	-3.182487000	-0.336249000	5.100135000
C	-4.301393000	-2.587665000	2.205186000
C	-4.751676000	-2.119592000	0.839266000
C	-3.713647000	-1.433879000	2.987693000
C	-6.184809000	-2.322906000	-1.128677000
C	1.623569000	-3.115148000	-3.586356000
H	0.690599000	-3.681346000	-3.711337000
H	2.265761000	-3.348382000	-4.449245000
H	1.376180000	-2.046259000	-3.608954000
C	2.271850000	3.579666000	-1.779674000
H	1.578624000	3.359445000	-2.607951000
C	4.647430000	-3.125407000	2.662371000
H	5.353658000	-3.184707000	3.492648000
C	3.907027000	1.410819000	-2.917367000
H	4.781188000	2.080998000	-2.876513000
C	-5.835746000	-2.704472000	0.173527000
H	-6.400205000	-3.489387000	0.679794000
C	4.979217000	0.518095000	1.844874000
C	0.176756000	-3.954988000	-0.205735000
H	0.618607000	-4.963774000	-0.209448000
C	4.048701000	-4.291158000	2.170576000
C	-3.829085000	-1.348677000	4.379215000
H	-4.416764000	-2.102740000	4.905502000
C	1.445703000	4.191543000	-0.635029000
H	0.642708000	3.514924000	-0.315220000
H	0.989842000	5.134280000	-0.974343000
H	2.081058000	4.416162000	0.231373000
C	-3.618601000	3.267190000	1.921251000
H	-3.756983000	2.707510000	0.988649000
H	-4.098727000	4.251077000	1.812881000
H	-4.131366000	2.718199000	2.722354000
C	-5.444626000	-1.316606000	-1.761774000
H	-5.705161000	-1.020498000	-2.777747000
C	4.863547000	-0.623473000	2.822925000
C	-4.531442000	2.174756000	-1.742902000
H	-4.927604000	2.093239000	-0.719065000
C	3.142058000	1.632324000	-4.237045000
H	2.204580000	1.061944000	-4.238123000
H	3.764193000	1.290985000	-5.078768000
H	2.904891000	2.690283000	-4.410917000
C	5.054450000	2.780883000	0.200429000
H	5.080327000	3.656510000	-0.444111000
C	0.259428000	1.895290000	3.182888000
H	-0.121742000	2.310698000	4.128698000
C	-2.559340000	-1.162222000	-3.803875000
H	-1.525644000	-1.149495000	-3.436827000
H	-2.534604000	-1.426945000	-4.872030000
H	-3.117137000	-1.943702000	-3.272800000
C	2.351934000	-3.510319000	-2.283702000
H	3.330438000	-3.004822000	-2.275638000
C	-1.006141000	-3.928906000	-1.193067000
H	-1.429007000	-2.917586000	-1.263717000
H	-1.800270000	-4.601017000	-0.835486000
H	-0.720593000	-4.253037000	-2.201353000
C	2.603376000	-5.028296000	-2.221333000
H	3.199905000	-5.310853000	-1.345507000
H	3.156856000	-5.343951000	-3.118698000
H	1.660580000	-5.593297000	-2.203018000
C	5.974758000	2.671298000	1.246366000
C	3.314672000	4.597085000	-2.292305000
H	3.917408000	4.997983000	-1.467502000
H	2.789603000	5.447375000	-2.753253000
H	3.994628000	4.178940000	-3.044368000
C	0.904827000	0.528085000	3.476811000
H	0.193675000	-0.174032000	3.928344000
H	1.738203000	0.672796000	4.181805000
H	1.300649000	0.079871000	2.558204000
C	-2.426285000	1.286787000	-4.431957000
H	-2.906789000	2.272886000	-4.403021000
H	-2.362136000	0.979106000	-5.486609000
H	-1.402945000	1.380665000	-4.047628000
C	-2.124005000	3.438466000	2.254434000
H	-1.662456000	4.062364000	1.472333000
C	1.301981000	2.865563000	2.605462000
H	1.720446000	2.460569000	1.675472000
H	2.130587000	2.990239000	3.318138000
H	0.883962000	3.859900000	2.395665000
C	-5.722061000	2.126142000	-2.717505000
H	-5.392490000	2.200001000	-3.763293000
H	-6.393031000	2.976725000	-2.523458000
H	-6.308858000	1.206596000	-2.599098000
C	4.411020000	-0.042521000	-2.822000000
H	4.934542000	-0.236810000	-1.877879000
H	5.103253000	-0.250980000	-3.652025000
H	3.569942000	-0.745201000	-2.906529000
C	-0.303684000	-3.625538000	1.220870000
H	0.509118000	-3.693399000	1.953546000
H	-1.090974000	-4.338174000	1.510821000
H	-0.721340000	-2.610991000	1.262095000
C	-1.958919000	4.146643000	3.612206000
H	-2.380298000	3.544516000	4.428827000
H	-2.507714000	5.100765000	3.592466000
H	-0.911995000	4.373091000	3.849551000
C	-3.760272000	3.506371000	-1.850270000
H	-2.879251000	3.508542000	-1.194415000
H	-4.416075000	4.341810000	-1.562851000
H	-3.416421000	3.692807000	-2.876461000
H	0.236339000	-0.252007000	0.626951000
H	-0.627874000	1.617207000	-1.504436000
H	5.831256000	-0.824272000	3.306730000
H	4.170638000	-0.334681000	3.637350000
H	4.288440000	-5.266086000	2.591887000
H	6.710230000	3.453491000	1.427847000
H	-7.016973000	-2.802671000	-1.641778000
H	-5.131959000	-3.053705000	2.754827000
H	-3.529378000	-3.371662000	2.084482000
H	-3.271065000	-0.284815000	6.184282000

$TS_{[2m-2]}$(open-shell singlet)

Ti	1.395728000	0.257741000	-0.789105000
Ti	-1.330290000	0.438386000	0.109538000
P	2.207790000	2.649672000	-0.212648000
P	-1.416791000	-0.554486000	2.598870000
P	-3.482935000	1.753269000	-0.641996000
P	2.090496000	-1.935943000	-1.909972000
N	-2.822305000	-1.028773000	0.018171000
N	3.330403000	-0.125954000	0.167968000
N	-0.425576000	0.927878000	-1.486455000
N	0.595249000	1.027784000	-2.321768000
C	-2.657734000	-2.227164000	0.742236000
C	3.699599000	2.250167000	0.756434000
C	4.943396000	-1.816019000	1.042943000
C	-1.773838000	-3.398412000	2.707759000
H	-1.215645000	-3.384678000	3.643094000
C	4.066087000	-3.670924000	-0.852537000
H	3.695521000	-4.401330000	-1.571562000
C	-3.975462000	-0.954261000	-0.790555000
C	3.908324000	-1.418700000	0.146968000
C	4.029196000	0.861699000	0.896526000
C	-3.472484000	2.838978000	-2.191324000
H	-4.522648000	3.118124000	-2.372020000

C	5.890374000	1.561020000	2.343772000
H	6.720327000	1.270856000	2.990947000
C	3.469844000	-2.396957000	-0.802487000
C	-1.952060000	-2.205232000	1.983344000
C	-4.506876000	0.317859000	-1.150991000
C	-2.323211000	-4.604881000	2.257898000
C	-3.960707000	-3.457538000	-1.018331000
C	-4.637561000	-2.123861000	-1.251380000
C	-3.224985000	-3.453129000	0.303453000
C	-6.369046000	-0.761102000	-2.306473000
C	2.022327000	-0.986105000	-4.633412000
H	1.363039000	-1.741182000	-5.083098000
H	2.632677000	-0.563768000	-5.446335000
H	1.400314000	-0.188598000	-4.207928000
C	1.189957000	3.965926000	0.697113000
H	0.309183000	4.050588000	0.039181000
C	5.541209000	-3.076744000	0.941852000
H	6.340573000	-3.327458000	1.641794000
C	2.894574000	3.571835000	-1.711113000
H	3.527350000	4.383529000	-1.316257000
C	-5.828617000	-2.012140000	-1.977016000
H	-6.325175000	-2.923706000	-2.314087000
C	5.106229000	0.550271000	1.779706000
C	1.049565000	-3.497464000	-2.093330000
H	1.651414000	-4.253627000	-2.622159000
C	5.116523000	-4.020549000	0.000060000
C	-3.062555000	-4.614072000	1.067243000
H	-3.509798000	-5.543933000	0.711790000
C	0.707121000	3.417236000	2.050217000
H	0.181719000	2.459014000	1.921190000
H	0.013979000	4.128700000	2.523597000
H	1.553505000	3.256936000	2.732205000
C	-4.165974000	-0.230633000	3.166651000
H	-4.184821000	0.263140000	2.188545000
H	-4.941156000	0.220333000	3.803852000
H	-4.423899000	-1.285879000	3.007662000
C	-5.689187000	0.396261000	-1.907848000
H	-6.078901000	1.371248000	-2.199833000
C	5.329598000	-0.889061000	2.168042000
C	-4.567662000	2.701136000	0.608909000
H	-5.025377000	1.885314000	1.186713000
C	1.772233000	4.161653000	-2.585522000
H	1.105542000	3.358906000	-2.929896000
H	2.209597000	4.651095000	-3.469103000
H	1.176974000	4.914742000	-2.050438000
C	4.511336000	3.243975000	1.336575000
H	4.273776000	4.290898000	1.159499000
C	0.055211000	-0.919447000	3.720913000
H	-0.320057000	-1.618921000	4.483781000
C	-2.958870000	2.065733000	-3.423446000
H	-1.915292000	1.755612000	-3.296932000
H	-3.022046000	2.718724000	-4.307439000
H	-3.562912000	1.170904000	-3.616462000
C	2.953872000	-1.617399000	-3.576462000
H	3.694948000	-0.856088000	-3.282234000
C	-0.220291000	-3.199537000	-2.918779000
H	-0.812788000	-2.406322000	-2.443081000
H	-0.840523000	-4.107164000	-2.973737000
H	0.006686000	-2.886742000	-3.944451000
C	3.715986000	-2.824329000	-4.154372000
H	4.456059000	-3.220371000	-3.448735000
H	4.249943000	-2.516632000	-5.066318000
H	3.028864000	-3.635413000	-4.436027000
C	5.625429000	2.916639000	2.112860000
C	1.797878000	5.373835000	0.862051000
H	2.577282000	5.384314000	1.634138000
H	1.009927000	6.071438000	1.184799000
H	2.225891000	5.765675000	-0.069365000
C	1.227721000	-1.591210000	2.983790000
H	0.920345000	-2.516231000	2.481725000
H	2.012937000	-1.840789000	3.714424000
H	1.655783000	-0.925602000	2.226108000
C	-2.657752000	4.130081000	-1.974798000
H	-3.048779000	4.741768000	-1.151105000
H	-2.685583000	4.741545000	-2.889028000
H	-1.606398000	3.896965000	-1.759348000
C	-2.788622000	-0.107182000	3.847360000
H	-2.607236000	0.954967000	4.078551000
C	0.521951000	0.364882000	4.436809000
H	0.942599000	1.077550000	3.717581000
H	1.310358000	0.116076000	5.162228000
H	-0.289762000	0.864666000	4.983779000
C	-5.710012000	3.543793000	0.011131000
H	-5.330479000	4.388695000	-0.579427000
H	-6.322764000	3.960711000	0.824756000
H	-6.371785000	2.943638000	-0.625879000
C	3.782048000	2.613997000	-2.531274000
H	4.571037000	2.163287000	-1.914991000
H	4.261444000	3.163972000	-3.355213000
H	3.172990000	1.812324000	-2.970526000
C	0.664835000	-4.038048000	-0.701127000
H	1.544760000	-4.338474000	-0.119981000
H	0.009311000	-4.914093000	-0.815364000
H	0.117854000	-3.277165000	-0.129422000
C	-2.779893000	-0.912940000	5.160045000
H	-2.874171000	-1.989401000	4.959816000
H	-3.641429000	-0.614338000	5.776606000
H	-1.874317000	-0.746006000	5.756760000
C	-3.696405000	3.530338000	1.575220000
H	-2.911699000	2.911522000	2.031543000
H	-4.319930000	3.950229000	2.379132000
H	-3.204216000	4.368302000	1.062661000
H	0.243915000	-0.561090000	0.408043000
H	-0.735797000	1.936577000	-0.849637000
H	6.373978000	-1.056035000	2.471603000
H	4.713379000	-1.122760000	3.058868000
H	5.578905000	-5.004776000	-0.055991000
H	6.254279000	3.693316000	2.545143000
H	-7.289202000	-0.690601000	-2.884523000
H	-4.686906000	-4.282229000	-1.060268000
H	-3.237854000	-3.637434000	-1.836835000
H	-2.187727000	-5.520027000	2.832342000

$TS_{[2m-2]}$(triplet)

Ti	1.482541000	0.311018000	-0.675936000
Ti	-1.331519000	0.403076000	0.140627000
P	2.530802000	2.601946000	-0.093150000
P	-1.671820000	-1.004945000	2.378732000
P	-3.280943000	2.089899000	-0.298650000
P	1.982711000	-1.925899000	-1.841627000
N	-3.020546000	-0.828509000	-0.211025000
N	3.394650000	-0.294667000	0.216179000
N	-0.360446000	0.891948000	-1.416603000
N	0.676149000	1.032988000	-2.223307000
C	-3.062747000	-2.145690000	0.287994000
C	4.077415000	2.035918000	0.691178000
C	4.815997000	-2.142339000	1.104790000
C	-2.457033000	-3.755459000	2.040483000
H	-1.948705000	-3.981291000	2.977852000
C	3.683005000	-3.919095000	-0.734314000
H	3.231424000	-4.607751000	-1.448469000
C	-4.117960000	-0.442781000	-1.001499000
C	3.815326000	-1.646447000	0.220854000
C	4.246014000	0.623627000	0.865122000
C	-3.122982000	3.481431000	-1.568120000
H	-4.136097000	3.896893000	-1.689121000
C	6.279155000	1.127914000	2.150197000
H	7.107050000	0.760080000	2.759357000

C	3.249420000	-2.581403000	-0.703290000
C	-2.413865000	-2.448211000	1.523326000
C	-4.460246000	0.937176000	-1.107790000
C	-3.159541000	-4.767696000	1.374542000
C	-4.437847000	-2.835479000	-1.694398000
C	-4.918850000	-1.399528000	-1.683349000
C	-3.782333000	-3.176091000	-0.373348000
C	-6.408470000	0.370748000	-2.468175000
C	2.234321000	-0.828232000	-4.515519000
H	1.621833000	-1.536171000	-5.090727000
H	2.947793000	-0.373087000	-5.219377000
H	1.580277000	-0.042500000	-4.117660000
C	1.710399000	3.839092000	1.085871000
H	0.743408000	4.024082000	0.590835000
C	5.244073000	-3.472658000	1.033474000
H	6.019961000	-3.804497000	1.725924000
C	3.090763000	3.631964000	-1.567436000
H	3.772270000	4.406506000	-1.180117000
C	-6.056900000	-0.984668000	-2.382133000
H	-6.662820000	-1.735463000	-2.892391000
C	5.325920000	0.209302000	1.702475000
C	0.834168000	-3.356700000	-2.270382000
H	1.419368000	-4.100413000	-2.834276000
C	4.686335000	-4.378636000	0.123994000
C	-3.829848000	-4.460195000	0.181253000
H	-4.389423000	-5.237491000	-0.342063000
C	1.422344000	3.147426000	2.431792000
H	0.839437000	2.229713000	2.280779000
H	0.847839000	3.822516000	3.084121000
H	2.357684000	2.887853000	2.946826000
C	-4.385632000	-0.549669000	3.035834000
H	-4.388190000	-0.013946000	2.079529000
H	-5.109982000	-0.070517000	3.711108000
H	-4.727051000	-1.574143000	2.838316000
C	-5.593299000	1.324029000	-1.845645000
H	-5.839270000	2.381378000	-1.943492000
C	5.356765000	-1.223629000	2.171734000
C	-4.247501000	2.849145000	1.155125000
H	-4.753094000	1.969305000	1.577474000
C	1.891595000	4.300028000	-2.266628000
H	1.184345000	3.534156000	-2.613761000
H	2.240508000	4.868455000	-3.142014000
H	1.361272000	4.999579000	-1.605702000
C	5.056152000	2.936595000	1.155797000
H	4.936475000	3.999518000	0.952111000
C	-0.244935000	-1.677817000	3.405647000
H	-0.680642000	-2.383981000	4.129154000
C	-2.654283000	2.942671000	-2.935625000
H	-1.652554000	2.501674000	-2.874400000
H	-2.622633000	3.773783000	-3.656598000
H	-3.338934000	2.178950000	-3.323578000
C	3.017764000	-1.552490000	-3.400060000
H	3.755996000	-0.844836000	-2.987596000
C	-0.332352000	-2.859280000	-3.152275000
H	-0.901460000	-2.075700000	-2.634270000
H	-1.013209000	-3.698700000	-3.359452000
H	0.005280000	-2.454264000	-4.112384000
C	3.782683000	-2.767032000	-3.958416000
H	4.406951000	-3.247883000	-3.195842000
H	4.439644000	-2.438784000	-4.778153000
H	3.093556000	-3.517285000	-4.372920000
C	6.181837000	2.494616000	1.854985000
C	2.415396000	5.192775000	1.297443000
H	3.334994000	5.074644000	1.884240000
H	1.749590000	5.862664000	1.862825000
H	2.666027000	5.694661000	0.353603000
C	0.794299000	-2.430786000	2.555807000
H	0.356044000	-3.301529000	2.054342000
H	1.608078000	-2.785135000	3.206727000
H	1.229167000	-1.773873000	1.792661000
C	-2.193316000	4.606569000	-1.073365000
H	-2.562513000	5.084502000	-0.156830000
H	-2.110349000	5.384039000	-1.847350000
H	-1.185133000	4.218555000	-0.875547000
C	-2.989278000	-0.564627000	3.690337000
H	-2.733208000	0.460727000	3.999450000
C	0.417278000	-0.519206000	4.180677000
H	0.877181000	0.190619000	3.481974000
H	1.208137000	-0.914181000	4.835379000
H	-0.296859000	0.029415000	4.811268000
C	-5.332309000	3.872897000	0.772549000
H	-4.899036000	4.787725000	0.345495000
H	-5.895384000	4.165035000	1.671890000
H	-6.049306000	3.457534000	0.053249000
C	3.871729000	2.736384000	-2.550123000
H	4.720973000	2.242611000	-2.059612000
H	4.261012000	3.345607000	-3.379756000
H	3.211367000	1.969097000	-2.975705000
C	0.277725000	-4.012561000	-0.991788000
H	1.070508000	-4.413027000	-0.349332000
H	-0.397130000	-4.836644000	-1.266242000
H	-0.303179000	-3.286435000	-0.408810000
C	-3.007695000	-1.470704000	4.935856000
H	-3.178412000	-2.520109000	4.656957000
H	-3.835195000	-1.165974000	5.594704000
H	-2.081073000	-1.410177000	5.520230000
C	-3.292997000	3.402623000	2.234392000
H	-2.528295000	2.662285000	2.506152000
H	-3.863306000	3.665460000	3.138256000
H	-2.773433000	4.308658000	1.894590000
H	0.413512000	0.157893000	0.843871000
H	-0.609789000	1.887807000	-0.663817000
H	6.374084000	-1.520468000	2.466941000
H	4.734061000	-1.316157000	3.084035000
H	5.020298000	-5.414431000	0.088905000
H	6.942460000	3.196789000	2.192445000
H	-7.288492000	0.679066000	-3.030522000
H	-5.262321000	-3.528257000	-1.916401000
H	-3.698379000	-2.957761000	-2.509344000
H	-3.191322000	-5.777296000	1.781477000

TS$_{[2m-3]}$(closed-shell singlet)

Ti	1.401798000	0.359758000	-0.612686000
Ti	-1.419150000	0.366244000	0.147447000
P	2.689425000	2.554229000	-0.048960000
P	-1.650078000	-0.962382000	2.398221000
P	-3.316089000	2.123441000	-0.191826000
P	1.857825000	-1.844913000	-1.863219000
N	-3.010706000	-0.823439000	-0.223254000
N	3.340402000	-0.384133000	0.217618000
N	-0.411774000	0.902299000	-1.276944000
N	0.621721000	1.119159000	-2.086569000
C	-3.078410000	-2.127504000	0.299360000
C	4.273249000	1.881422000	0.546114000
C	4.688336000	-2.319015000	1.032353000
C	-2.469631000	-3.710090000	2.059012000
H	-1.955308000	-3.937851000	2.992066000
C	3.432944000	-3.988848000	-0.830500000
H	2.944947000	-4.631890000	-1.563077000
C	-4.012724000	-0.427981000	-1.122375000
C	3.694113000	-1.755609000	0.183501000
C	4.318154000	0.469152000	0.768759000
C	-3.010143000	3.623490000	-1.304309000
H	-3.997704000	4.061419000	-1.516793000
C	6.476256000	0.815179000	1.890219000
H	7.305406000	0.392422000	2.460646000
C	3.073196000	-2.631447000	-0.757982000
C	-2.419432000	-2.404312000	1.535248000

C	-4.278406000	0.964707000	-1.269588000
C	-3.189335000	-4.719948000	1.407177000
C	-4.415286000	-2.844279000	-1.716404000
C	-4.771629000	-1.375359000	-1.851684000
C	-3.793343000	-3.153400000	-0.366889000
C	-6.003839000	0.440980000	-2.918491000
C	2.114539000	3.755672000	1.305262000
H	1.048823000	3.908751000	1.073919000
C	5.040155000	-3.669325000	0.927280000
H	5.810121000	-4.058674000	1.595811000
C	3.111322000	3.633710000	-1.531455000
H	3.831335000	4.389947000	-1.179168000
C	-5.768095000	-0.928135000	-2.728057000
H	-6.349665000	-1.662250000	-3.288146000
C	5.407388000	-0.019190000	1.553156000
C	0.622209000	-3.169228000	-2.368777000
H	1.163563000	-3.907792000	-2.981541000
C	4.417116000	-4.522063000	0.008045000
C	-3.856116000	-4.429145000	0.207425000
H	-4.422139000	-5.211023000	-0.301844000
C	-5.253577000	1.378457000	-2.196535000
H	-5.439758000	2.440712000	-2.350694000
C	5.313699000	-1.430258000	2.077833000
C	-4.681353000	2.728891000	1.021764000
H	-5.233411000	1.797314000	1.215831000
C	5.363486000	2.699685000	0.901647000
H	5.327550000	3.762927000	0.666673000
C	-0.229880000	-1.698935000	3.406546000
H	-0.665834000	-2.433401000	4.100407000
C	2.921355000	-1.441907000	-3.391869000
H	3.672145000	-0.769795000	-2.944819000
C	6.491385000	2.172367000	1.536244000
C	-2.938131000	-0.567450000	3.767227000
H	-2.648210000	0.435455000	4.120685000
H	-0.587858000	2.768392000	3.109534000
H	-1.186060000	2.664002000	2.685004000
H	-6.768869000	0.774336000	-3.618359000
H	-5.301228000	-3.474272000	-1.886540000
H	-3.235139000	-5.721901000	1.831755000
H	-3.694851000	-3.111748000	-2.512464000
H	4.692888000	-5.573581000	-0.054599000
H	6.300525000	-1.808912000	2.381192000
H	4.684668000	-1.433838000	2.990332000
H	7.340271000	2.806615000	1.786208000
C	2.219550000	3.050020000	2.671822000
H	3.270424000	2.907084000	2.954851000
H	1.733396000	3.659761000	3.448092000
H	1.736912000	2.064090000	2.654362000
C	2.803524000	5.133412000	1.352154000
H	2.318151000	5.753265000	2.121470000
H	3.862099000	5.041296000	1.626648000
H	2.736118000	5.674162000	0.399904000
C	1.852443000	4.331238000	-2.080983000
H	1.375657000	4.982115000	-1.334853000
H	2.121940000	4.955483000	-2.946196000
H	1.122535000	3.579246000	-2.408247000
C	3.786574000	2.777438000	-2.621206000
H	4.684923000	2.273964000	-2.240544000
H	3.087636000	2.020287000	-2.999204000
H	4.082608000	3.418937000	-3.464926000
C	2.167110000	-0.657791000	-4.485834000
H	2.897454000	-0.177175000	-5.154201000
H	1.558347000	-1.331653000	-5.104357000
H	1.514873000	0.115799000	-4.060727000
C	3.657616000	-2.657885000	-3.984711000
H	4.331892000	-2.320494000	-4.786355000
H	4.259184000	-3.182791000	-3.233151000
H	2.951811000	-3.373470000	-4.431428000
C	-0.514784000	-2.551969000	-3.212247000
H	-0.155758000	-2.115033000	-4.150071000
H	-1.244381000	-3.336815000	-3.462966000
H	-1.034065000	-1.765200000	-2.648825000
C	0.037978000	-3.872687000	-1.127836000
H	0.808296000	-4.374364000	-0.531188000
H	-0.476886000	-3.151142000	-0.480950000
H	-0.699503000	-4.624351000	-1.445381000
C	-2.165680000	4.673141000	-0.552459000
H	-1.998663000	5.548798000	-1.197459000
H	-2.652505000	5.023633000	0.367522000
H	-1.184053000	4.258144000	-0.285665000
C	-2.349205000	3.243396000	-2.643087000
H	-2.220929000	4.154406000	-3.248444000
H	-1.368162000	2.781186000	-2.491392000
H	-2.966810000	2.538768000	-3.212953000
C	-5.681262000	3.755678000	0.458795000
H	-6.153616000	3.407388000	-0.467930000
H	-6.482753000	3.925757000	1.194126000
H	-5.204244000	4.726713000	0.265883000
C	-4.088179000	3.211940000	2.358447000
H	-3.503302000	4.134385000	2.237813000
H	-4.897721000	3.424255000	3.073271000
H	-3.433916000	2.451339000	2.801659000
C	0.439082000	-0.578513000	4.227831000
H	-0.266921000	-0.061554000	4.893137000
H	1.244432000	-0.996357000	4.849761000
H	0.885800000	0.166617000	3.555343000
C	0.802010000	-2.407801000	2.515601000
H	1.196469000	-1.716136000	1.757336000
H	1.643149000	-2.764290000	3.129678000
H	0.367823000	-3.270025000	1.995314000
C	-4.335539000	-0.475524000	3.124976000
H	-4.312849000	0.104892000	2.194543000
H	-4.712773000	-1.477793000	2.881680000
H	-5.044246000	-0.000967000	3.820007000
C	-2.974142000	-1.526797000	4.971110000
H	-3.782128000	-1.225630000	5.656036000
H	-3.184966000	-2.556091000	4.648097000
H	-2.038991000	-1.526140000	5.545149000

TS$_{[2m-3]}$(open-shell singlet)

Ti	1.426600000	0.381919000	-0.612995000
Ti	-1.410269000	0.389336000	0.174384000
P	2.763067000	2.517426000	0.042819000
P	-1.627030000	-1.015072000	2.391691000
P	-3.252419000	2.186717000	-0.211868000
P	1.764513000	-1.796883000	-1.926306000
N	-3.054684000	-0.792460000	-0.162722000
N	3.331451000	-0.456891000	0.181180000
N	-0.393012000	0.922809000	-1.260977000
N	0.624427000	1.174552000	-2.067430000
C	-3.205201000	-2.085805000	0.377830000
C	4.325517000	1.767568000	0.607236000
C	4.619090000	-2.465443000	0.911381000
C	-2.709303000	-3.681784000	2.167115000
H	-2.206939000	-3.925566000	3.103005000
C	3.267778000	-4.029392000	-0.975647000
H	2.741543000	-4.631605000	-1.716406000
C	-4.034661000	-0.365144000	-1.077648000
C	3.634974000	-1.838664000	0.096405000
C	4.335714000	0.344903000	0.761934000
C	-2.934311000	3.675545000	-1.332750000
H	-3.915867000	4.131513000	-1.536275000
C	6.512009000	0.581867000	1.877373000
H	7.334622000	0.110855000	2.418771000
C	2.965130000	-2.661135000	-0.860768000
C	-2.565568000	-2.396888000	1.614278000
C	-4.246726000	1.034825000	-1.260367000
C	-3.496342000	-4.653392000	1.534244000

C	-4.551835000	-2.767029000	-1.640152000
C	-4.837085000	-1.286918000	-1.798142000
C	-3.979607000	-3.079712000	-0.271969000
C	-5.996249000	0.557810000	-2.899328000
C	2.249199000	3.726645000	1.416536000
H	1.184475000	3.909206000	1.203302000
C	4.914618000	-3.825365000	0.762106000
H	5.678936000	-4.264031000	1.406197000
C	3.224585000	3.602832000	-1.425813000
H	3.970819000	4.328938000	-1.065015000
C	-5.814209000	-0.815011000	-2.682076000
H	-6.425076000	-1.536828000	-3.226889000
C	5.418821000	-0.207652000	1.511511000
C	0.480588000	-3.064238000	-2.461033000
H	0.993942000	-3.810495000	-3.088297000
C	4.242426000	-4.625881000	-0.169014000
C	-4.129474000	-4.338705000	0.323636000
H	-4.735967000	-5.091625000	-0.182875000
C	-5.205114000	1.472363000	-2.193934000
H	-5.344850000	2.539309000	-2.364657000
C	5.295148000	-1.637624000	1.975360000
C	-4.564237000	2.805613000	1.039893000
H	-5.100185000	1.874278000	1.276263000
C	5.440356000	2.538651000	0.990803000
H	5.430174000	3.612489000	0.807581000
C	-0.185373000	-1.840892000	3.286647000
H	-0.607941000	-2.534192000	4.029592000
C	2.831474000	-1.404623000	-3.458461000
H	3.619128000	-0.783032000	-3.001488000
C	6.559570000	1.953459000	1.588697000
C	-2.764350000	-0.482359000	3.836870000
H	-2.374932000	0.504965000	4.132759000
H	-0.579511000	2.211729000	2.436680000
H	-0.786917000	2.835352000	2.784279000
H	-6.747106000	0.910015000	-3.605113000
H	-5.459778000	-3.359363000	-1.827694000
H	-3.610691000	-5.642596000	1.975265000
H	-3.821145000	-3.075528000	-2.412151000
H	4.473751000	-5.685565000	-0.265385000
H	6.277517000	-2.056704000	2.237703000
H	4.689655000	-1.662989000	2.903491000
H	7.426436000	2.553358000	1.860825000
C	2.356648000	3.017687000	2.781096000
H	3.408204000	2.860012000	3.053367000
H	1.884471000	3.633175000	3.561144000
H	1.858603000	2.040141000	2.769446000
C	2.973281000	5.087082000	1.456395000
H	2.516459000	5.714482000	2.237064000
H	4.034039000	4.969683000	1.712177000
H	2.902594000	5.634618000	0.508391000
C	1.990584000	4.349822000	-1.967073000
H	1.534091000	5.005283000	-1.212322000
H	2.281613000	4.977220000	-2.823054000
H	1.235991000	3.627749000	-2.306089000
C	3.869151000	2.737296000	-2.526825000
H	4.748617000	2.196813000	-2.153081000
H	3.144179000	2.010694000	-2.916452000
H	4.187981000	3.378112000	-3.362726000
C	2.107426000	-0.553816000	-4.522793000
H	2.854688000	-0.083581000	-5.179893000
H	1.467435000	-1.180505000	-5.159142000
H	1.489949000	0.232346000	-4.069885000
C	3.503013000	-2.635949000	-4.094933000
H	4.184566000	-2.307438000	-4.894243000
H	4.086677000	-3.210903000	-3.366219000
H	2.759513000	-3.303716000	-4.554349000
C	-0.632689000	-2.387553000	-3.290534000
H	-0.258826000	-1.946249000	-4.220562000
H	-1.392416000	-3.138619000	-3.555330000
H	-1.120591000	-1.593586000	-2.709391000
C	-0.132981000	-3.768715000	-1.235958000
H	0.617836000	-4.301535000	-0.641361000
H	-0.630631000	-3.039674000	-0.583580000
H	-0.890685000	-4.493303000	-1.569092000
C	-2.059308000	4.714053000	-0.599909000
H	-1.877716000	5.576413000	-1.258569000
H	-2.531020000	5.088971000	0.318056000
H	-1.085561000	4.280070000	-0.335642000
C	-2.294065000	3.273354000	-2.675893000
H	-2.159007000	4.177593000	-3.289711000
H	-1.317492000	2.799239000	-2.530918000
H	-2.927631000	2.573621000	-3.233926000
C	-5.592655000	3.810427000	0.489195000
H	-6.092142000	3.435217000	-0.412625000
H	-6.369631000	3.991020000	1.247681000
H	-5.130610000	4.780174000	0.257322000
C	-3.920842000	3.323723000	2.341170000
H	-3.365837000	4.257818000	2.178087000
H	-4.702548000	3.529454000	3.087986000
H	-3.227185000	2.587532000	2.764673000
C	0.641438000	-0.765712000	4.019952000
H	0.042258000	-0.185007000	4.735536000
H	1.465247000	-1.238545000	4.574826000
H	1.080308000	-0.068226000	3.293095000
C	0.698583000	-2.635474000	2.312317000
H	1.068771000	-1.984887000	1.506439000
H	1.570123000	-3.045162000	2.844424000
H	0.151230000	-3.468292000	1.855329000
C	-4.200544000	-0.305984000	3.307049000
H	-4.217505000	0.259873000	2.367952000
H	-4.661039000	-1.283883000	3.113755000
H	-4.816172000	0.224597000	4.048571000
C	-2.768151000	-1.404158000	5.070500000
H	-3.483655000	-1.017876000	5.812871000
H	-3.090030000	-2.420205000	4.802513000
H	-1.787610000	-1.466165000	5.558966000

$TS_{[2m-3]}$(triplet)

Ti	1.429231000	0.392550000	-0.646864000
Ti	-1.416095000	0.430399000	0.192211000
P	2.731308000	2.536929000	0.026193000
P	-1.514370000	-0.963722000	2.407999000
P	-3.356269000	2.140364000	-0.256756000
P	1.752533000	-1.791093000	-1.944242000
N	-3.034373000	-0.830229000	-0.103954000
N	3.333775000	-0.433804000	0.155742000
N	-0.380558000	0.970947000	-1.247612000
N	0.618320000	1.200962000	-2.083414000
C	-3.158811000	-2.103793000	0.490752000
C	4.292254000	1.799852000	0.615435000
C	4.642293000	-2.434467000	0.869591000
C	-2.635941000	-3.617030000	2.346013000
H	-2.121131000	-3.814157000	3.286228000
C	3.289496000	-4.004446000	-1.010468000
H	2.759592000	-4.609771000	-1.746014000
C	-4.035767000	-0.465596000	-1.025778000
C	3.648809000	-1.812189000	0.062206000
C	4.323561000	0.375200000	0.751971000
C	-3.079380000	3.606746000	-1.416035000
H	-4.070101000	4.038288000	-1.628254000
C	6.489256000	0.630655000	1.884471000
H	7.316100000	0.164414000	2.423590000
C	2.976844000	-2.638703000	-0.891046000
C	-2.501635000	-2.360019000	1.730264000
C	-4.298934000	0.918150000	-1.263810000
C	-3.425216000	-4.620953000	1.769629000
C	-4.495023000	-2.899667000	-1.489307000
C	-4.817095000	-1.436147000	-1.707274000

C	-3.925996000	-3.136882000	-0.106085000
C	-6.038650000	0.326160000	-2.875658000
C	2.202318000	3.784513000	1.360188000
H	1.144985000	3.969355000	1.114750000
C	4.948473000	-3.791306000	0.713765000
H	5.720326000	-4.225437000	1.351968000
C	3.212572000	3.595971000	-1.457317000
H	3.959558000	4.323878000	-1.101694000
C	-5.811816000	-1.030026000	-2.603374000
H	-6.402316000	-1.792647000	-3.114037000
C	5.411738000	-0.170926000	1.498498000
C	0.470102000	-3.071188000	-2.453315000
H	0.978384000	-3.816350000	-3.085898000
C	4.276347000	-4.594979000	-0.214533000
C	-4.064028000	-4.367696000	0.548067000
H	-4.664285000	-5.148396000	0.077429000
C	-5.274815000	1.289856000	-2.208134000
H	-5.447937000	2.345162000	-2.417088000
C	5.313113000	-1.609935000	1.939480000
C	-4.680357000	2.736158000	0.987694000
H	-5.156403000	1.786133000	1.273960000
C	5.392409000	2.582053000	1.018258000
H	5.368000000	3.657537000	0.847776000
C	-0.035058000	-1.773957000	3.252612000
H	-0.427165000	-2.408316000	4.061944000
C	2.793802000	-1.408354000	-3.498243000
H	3.590497000	-0.785696000	-3.058535000
C	6.515965000	2.006877000	1.617648000
C	-2.566258000	-0.356370000	3.887780000
H	-2.164377000	0.645898000	4.106950000
H	-0.631938000	2.333556000	2.259565000
H	-0.923714000	2.987361000	2.461961000
H	-6.801352000	0.626524000	-3.592512000
H	-5.385336000	-3.523088000	-1.659161000
H	-3.532276000	-5.588018000	2.258883000
H	-3.748886000	-3.219581000	-2.241735000
H	4.515482000	-5.652498000	-0.315521000
H	6.303873000	-2.017283000	2.188814000
H	4.715468000	-1.659665000	2.871815000
H	7.370602000	2.616955000	1.905455000
C	2.267618000	3.113347000	2.745692000
H	3.309899000	2.941584000	3.044412000
H	1.793589000	3.760830000	3.498440000
H	1.749098000	2.146768000	2.751964000
C	2.932671000	5.142362000	1.384973000
H	2.451209000	5.794763000	2.129615000
H	3.982751000	5.029026000	1.682750000
H	2.899218000	5.661900000	0.419467000
C	1.987767000	4.339461000	-2.023957000
H	1.529917000	5.014154000	-1.286998000
H	2.289383000	4.946427000	-2.891019000
H	1.231058000	3.614718000	-2.353107000
C	3.863824000	2.708841000	-2.536847000
H	4.733327000	2.165986000	-2.143579000
H	3.137452000	1.983376000	-2.926222000
H	4.199657000	3.333974000	-3.377994000
C	2.052848000	-0.561051000	-4.553798000
H	2.789114000	-0.095840000	-5.226734000
H	1.399777000	-1.189096000	-5.175329000
H	1.445629000	0.229290000	-4.094316000
C	3.453679000	-2.642239000	-4.141893000
H	4.120784000	-2.317207000	-4.954755000
H	4.050686000	-3.214122000	-3.421611000
H	2.702127000	-3.311921000	-4.585097000
C	-0.658825000	-2.402462000	-3.267830000
H	-0.300843000	-1.959514000	-4.203311000
H	-1.418024000	-3.157867000	-3.521545000
H	-1.142945000	-1.611356000	-2.679570000
C	-0.122453000	-3.774685000	-1.217564000
H	0.639606000	-4.299855000	-0.630332000
H	-0.617595000	-3.046012000	-0.562749000
H	-0.878057000	-4.506955000	-1.538912000
C	-2.218264000	4.679545000	-0.716328000
H	-2.052952000	5.525250000	-1.400244000
H	-2.692121000	5.073607000	0.192388000
H	-1.236786000	4.267674000	-0.444756000
C	-2.433228000	3.178503000	-2.748798000
H	-2.306638000	4.068688000	-3.384317000
H	-1.451297000	2.719953000	-2.588813000
H	-3.057877000	2.458363000	-3.290602000
C	-5.771742000	3.652675000	0.405543000
H	-6.256907000	3.206800000	-0.471437000
H	-6.549862000	3.823084000	1.165048000
H	-5.368916000	4.635431000	0.123455000
C	-4.054244000	3.352012000	2.254938000
H	-3.561831000	4.310649000	2.042015000
H	-4.839029000	3.543017000	3.002280000
H	-3.312103000	2.680753000	2.703496000
C	0.863743000	-0.681215000	3.864215000
H	0.322353000	-0.029982000	4.565202000
H	1.700242000	-1.143004000	4.409458000
H	1.285762000	-0.054326000	3.066544000
C	0.765700000	-2.654679000	2.280038000
H	1.118794000	-2.067675000	1.420740000
H	1.648582000	-3.067092000	2.790848000
H	0.165308000	-3.489840000	1.900875000
C	-4.030720000	-0.209273000	3.430287000
H	-4.102295000	0.304371000	2.463661000
H	-4.497782000	-1.196368000	3.315907000
H	-4.606121000	0.361280000	4.174426000
C	-2.497402000	-1.207869000	5.168961000
H	-3.169308000	-0.779602000	5.928812000
H	-2.832130000	-2.237095000	4.978142000
H	-1.489978000	-1.243340000	5.602448000

TS$_{[H'-I]}$(closed-shell singlet)

Ti	1.409704000	0.375756000	-0.580246000
Ti	-1.383001000	0.109213000	-0.140881000
P	2.388392000	2.253818000	0.964227000
P	-1.670582000	-1.422834000	2.055739000
P	-3.266122000	1.988547000	-0.387297000
P	2.766106000	-0.596706000	-2.598516000
N	-3.210083000	-0.972134000	-0.430251000
N	3.091330000	-0.550345000	0.362334000
N	-0.252022000	0.326552000	-1.603765000
N	-0.130869000	1.501100000	-0.696824000
C	-3.391681000	-2.279596000	0.048917000
C	3.441896000	1.215614000	2.042409000
C	4.390993000	-2.655828000	0.567468000
C	-2.939107000	-3.984598000	1.755747000
H	-2.426550000	-4.295497000	2.665753000
C	4.200601000	-3.043767000	-2.204532000
H	4.120115000	-3.200176000	-3.280092000
C	-4.243444000	-0.467239000	-1.240812000
C	3.686158000	-1.698521000	-0.211198000
C	3.622745000	-0.133751000	1.602729000
C	-2.882410000	3.389176000	-1.596517000
H	-3.836050000	3.906245000	-1.789805000
C	4.983557000	-0.530172000	3.597926000
H	5.566964000	-1.223685000	4.206359000
C	3.619036000	-1.900629000	-1.626073000
C	-2.734158000	-2.687186000	1.249252000
C	-4.448653000	0.941733000	-1.325201000
C	-3.797718000	-4.883994000	1.113605000
C	-4.806969000	-2.807807000	-1.955093000
C	-5.114861000	-1.326239000	-1.964888000
C	-4.228872000	-3.217002000	-0.618181000
C	-6.361918000	0.595597000	-2.807932000

C	3.751395000	1.801657000	-3.814559000
H	3.217532000	1.722175000	-4.769973000
H	4.627435000	2.447059000	-3.977552000
H	3.084586000	2.300019000	-3.098523000
C	1.112880000	3.138998000	2.046973000
H	0.381183000	3.478153000	1.297558000
C	4.994389000	-3.760286000	-0.045464000
H	5.533974000	-4.474509000	0.578991000
C	3.525020000	3.644765000	0.382295000
H	3.814021000	4.210410000	1.282072000
C	-6.166584000	-0.790306000	-2.713869000
H	-6.826235000	-1.470526000	-3.255697000
C	4.372652000	-1.011269000	2.434774000
C	1.985212000	-1.492762000	-4.060098000
H	2.788897000	-1.986863000	-4.628806000
C	4.894777000	-3.976381000	-1.425650000
C	-4.436831000	-4.486117000	-0.070456000
H	-5.093448000	-5.183326000	-0.594069000
C	0.407821000	2.112772000	2.952742000
H	0.021796000	1.267417000	2.363068000
H	-0.437272000	2.589421000	3.471057000
H	1.095827000	1.714307000	3.710365000
C	-4.135209000	-0.429149000	2.986988000
H	-4.072415000	0.178394000	2.077007000
H	-4.689201000	0.134283000	3.752525000
H	-4.708630000	-1.332669000	2.741115000
C	-5.490402000	1.450124000	-2.124357000
H	-5.621180000	2.528063000	-2.216106000
C	4.420640000	-2.477743000	2.068785000
C	-4.349244000	2.797588000	0.966042000
H	-4.984108000	1.958784000	1.287628000
C	2.771163000	4.581634000	-0.582981000
H	2.430633000	4.035350000	-1.472791000
H	3.435028000	5.395060000	-0.911963000
H	1.887511000	5.036245000	-0.115546000
C	4.060241000	1.663159000	3.224504000
H	3.940189000	2.701959000	3.529046000
C	-0.336632000	-2.442108000	2.920989000
H	-0.860522000	-3.128607000	3.603574000
C	-2.344256000	2.838259000	-2.932732000
H	-1.416364000	2.275989000	-2.775238000
H	-2.137055000	3.681799000	-3.609890000
H	-3.072856000	2.179057000	-3.421062000
C	4.208689000	0.420731000	-3.298977000
H	4.817831000	0.578767000	-2.395283000
C	1.255519000	-0.491651000	-4.981911000
H	0.517931000	0.087664000	-4.410789000
H	0.722572000	-1.044254000	-5.770173000
H	1.945985000	0.203425000	-5.475537000
C	5.072984000	-0.315768000	-4.337969000
H	5.438636000	-1.276505000	-3.953861000
H	5.949323000	0.298652000	-4.594391000
H	4.515934000	-0.498590000	-5.267626000
C	4.845497000	0.805034000	4.001810000
C	1.581149000	4.358717000	2.864458000
H	2.293378000	4.074303000	3.650335000
H	0.711241000	4.813406000	3.362775000
H	2.044885000	5.135032000	2.242874000
C	0.484464000	-3.277616000	1.922747000
H	-0.147904000	-3.952365000	1.332900000
H	1.217224000	-3.888175000	2.472332000
H	1.033420000	-2.622442000	1.233126000
C	-1.882843000	4.391393000	-0.984548000
H	-2.262542000	4.856503000	-0.064394000
H	-1.683563000	5.198699000	-1.706161000
H	-0.938550000	3.876426000	-0.767201000
C	-2.737740000	-0.807609000	3.515293000
H	-2.230291000	0.107152000	3.861123000
C	0.588706000	-1.532729000	3.752538000
H	1.160046000	-0.863308000	3.097379000
H	1.308330000	-2.146936000	4.314070000
H	0.037460000	-0.917680000	4.477351000
C	-5.276711000	3.933741000	0.496961000
H	-4.708215000	4.811162000	0.159598000
H	-5.914700000	4.256350000	1.334247000
H	-5.937882000	3.612427000	-0.317136000
C	4.806320000	3.080773000	-0.257635000
H	5.363225000	2.451433000	0.447481000
H	5.458753000	3.908625000	-0.573741000
H	4.570927000	2.477247000	-1.142700000
C	0.990996000	-2.559255000	-3.558834000
H	1.464117000	-3.286650000	-2.887183000
H	0.577874000	-3.105560000	-4.420113000
H	0.159967000	-2.080074000	-3.028139000
C	-2.871541000	-1.782730000	4.699978000
H	-3.309861000	-2.736597000	4.374707000
H	-3.547107000	-1.349427000	5.453493000
H	-1.913962000	-1.988429000	5.194424000
C	-3.495366000	3.236258000	2.173536000
H	-2.864163000	2.414898000	2.536480000
H	-4.147855000	3.559388000	2.999067000
H	-2.837719000	4.078920000	1.920525000
H	-0.895130000	-2.524524000	-0.835245000
H	-0.331707000	-2.056632000	-0.665896000
H	-7.172213000	1.000538000	-3.412565000
H	-5.700667000	-3.400396000	-2.198791000
H	-4.063853000	-3.024034000	-2.747790000
H	-3.957486000	-5.881350000	1.520685000
H	3.545281000	-2.988028000	2.513737000
H	5.308927000	-2.961157000	2.501546000
H	5.351586000	-4.851507000	-1.885262000
H	5.329738000	1.163890000	4.908742000

$TS_{[H'-1]}$(triplet)

Ti	1.607575000	0.664896000	-0.106117000
Ti	-1.610290000	0.123574000	-0.071292000
P	2.946229000	0.889743000	2.145090000
P	-1.977634000	-2.316467000	0.790579000
P	-3.098685000	2.038047000	0.856101000
P	2.733137000	1.268423000	-2.396942000
N	-3.605730000	-0.358057000	-0.745568000
N	3.115696000	-0.801442000	-0.293955000
N	-0.160753000	1.176163000	-0.724832000
N	-0.062495000	0.926519000	0.764414000
C	-3.958214000	-1.680481000	-1.065417000
C	3.817026000	-0.725439000	2.066386000
C	4.024192000	-2.586817000	-1.752934000
C	-3.632418000	-4.092767000	-0.739937000
H	-3.098604000	-4.916555000	-0.266970000
C	3.689471000	-0.923191000	-3.988582000
H	3.555017000	-0.283188000	-4.860305000
C	-4.592094000	0.619232000	-0.976524000
C	3.484227000	-1.287000000	-1.569470000
C	3.742765000	-1.413363000	0.814394000
C	-2.525377000	3.812637000	0.568853000
H	-3.368478000	4.470599000	0.835228000
C	5.056885000	-3.226446000	1.797552000
H	5.520115000	-4.208839000	1.689159000
C	3.341736000	-0.441331000	-2.713788000
C	-3.280666000	-2.765634000	-0.427859000
C	-4.541641000	1.851335000	-0.258225000
C	-4.663816000	-4.375862000	-1.642686000
C	-5.617306000	-0.830374000	-2.755976000
C	-5.656933000	0.413624000	-1.895402000
C	-4.985514000	-1.981215000	-2.002809000
C	-6.602003000	2.597192000	-1.337949000
C	4.165596000	3.671790000	-1.781070000
H	3.638905000	4.352063000	-2.462485000

H	5.149045000	4.115948000	-1.566238000
H	3.594325000	3.625850000	-0.844152000
C	1.850290000	0.894521000	3.692892000
H	1.190864000	1.755562000	3.501637000
C	4.397616000	-3.020416000	-3.030903000
H	4.812635000	-4.023499000	-3.143482000
C	4.314046000	2.124951000	2.563506000
H	4.703778000	1.844297000	3.554482000
C	-6.651523000	1.385766000	-2.043362000
H	-7.464210000	1.201226000	-2.748381000
C	4.342371000	-2.698908000	0.715894000
C	1.800422000	1.750801000	-3.959552000
H	2.490967000	1.647873000	-4.811611000
C	4.221165000	-2.207582000	-4.157530000
C	-5.335527000	-3.310940000	-2.259516000
H	-6.132475000	-3.514027000	-2.977198000
C	0.965371000	-0.366665000	3.710460000
H	0.399728000	-0.459794000	2.775047000
H	0.247720000	-0.299325000	4.542344000
H	1.571827000	-1.271181000	3.855425000
C	-4.089561000	-1.970325000	2.616275000
H	-3.973366000	-0.908842000	2.367333000
H	-4.468431000	-2.049709000	3.646142000
H	-4.843482000	-2.393307000	1.938795000
C	-5.533888000	2.827106000	-0.463253000
H	-5.469891000	3.778732000	0.064327000
C	4.118039000	-3.498270000	-0.549142000
C	-3.843518000	2.008122000	2.607276000
H	-4.566033000	1.181491000	2.528930000
C	3.734272000	3.551700000	2.633582000
H	3.302247000	3.843443000	1.666031000
H	4.528448000	4.270791000	2.883896000
H	2.945866000	3.643424000	3.392946000
C	4.536021000	-1.290216000	3.135463000
H	4.617136000	-0.742251000	4.073106000
C	-0.674893000	-3.664815000	0.576636000
H	-1.182361000	-4.631286000	0.718715000
C	-2.179639000	4.027046000	-0.918666000
H	-1.355956000	3.362717000	-1.212112000
H	-1.867246000	5.071623000	-1.072529000
H	-3.041301000	3.828115000	-1.569073000
C	4.348401000	2.270184000	-2.400546000
H	4.969352000	1.674081000	-1.713218000
C	1.315781000	3.214576000	-3.890003000
H	0.705850000	3.380676000	-2.992507000
H	0.692933000	3.433927000	-4.770075000
H	2.146644000	3.930734000	-3.886120000
C	5.066019000	2.339299000	-3.760376000
H	5.243041000	1.339584000	-4.176621000
H	6.043142000	2.831449000	-3.640980000
H	4.489765000	2.925861000	-4.489926000
C	5.170913000	-2.531469000	3.008956000
C	2.541871000	1.098405000	5.055137000
H	3.183477000	0.246519000	5.316455000
H	1.772528000	1.178125000	5.838219000
H	3.147366000	2.012830000	5.096639000
C	-0.076461000	-3.633399000	-0.842129000
H	-0.849789000	-3.742504000	-1.612626000
H	0.642732000	-4.458228000	-0.959596000
H	0.459789000	-2.690770000	-1.020041000
C	-1.313699000	4.157033000	1.460078000
H	-1.566249000	4.138638000	2.528753000
H	-0.959454000	5.171548000	1.220158000
H	-0.496573000	3.445783000	1.283605000
C	-2.755279000	-2.728362000	2.483188000
H	-2.040881000	-2.310541000	3.210427000
C	0.430585000	-3.528445000	1.641379000
H	0.970620000	-2.580722000	1.522148000
H	1.159394000	-4.345112000	1.530814000
H	0.035176000	-3.569986000	2.665379000
C	-4.617401000	3.273663000	3.020511000
H	-3.953538000	4.144815000	3.107596000
H	-5.084690000	3.115729000	4.004659000
H	-5.417018000	3.514011000	2.308707000
C	5.470608000	2.034262000	1.551972000
H	5.910987000	1.029674000	1.535226000
H	6.258521000	2.753296000	1.822458000
H	5.126752000	2.275326000	0.538333000
C	0.600011000	0.805862000	-4.162362000
H	0.909302000	-0.245117000	-4.226172000
H	0.079871000	1.068078000	-5.096198000
H	-0.105490000	0.912363000	-3.329659000
C	-2.959028000	-4.225347000	2.780801000
H	-3.638337000	-4.682123000	2.048189000
H	-3.418179000	-4.342145000	3.774604000
H	-2.018108000	-4.790497000	2.784393000
C	-2.785727000	1.617561000	3.659948000
H	-2.229449000	0.723057000	3.351527000
H	-3.276063000	1.413601000	4.624162000
H	-2.057120000	2.423316000	3.819147000
H	-1.689163000	-1.214206000	-2.486835000
H	-0.986901000	-0.991926000	-2.372885000
H	-7.373519000	3.352501000	-1.480355000
H	-6.623338000	-1.097709000	-3.111307000
H	-5.016347000	-0.619920000	-3.662765000
H	-4.934105000	-5.406516000	-1.867787000
H	3.173859000	-4.068014000	-0.451390000
H	4.913059000	-4.245940000	-0.686386000
H	4.495895000	-2.565919000	-5.148462000
H	5.733021000	-2.953917000	3.840450000

$TS_{[H'-2]}$(closed-shell singlet)

Ti	1.476327000	0.246888000	-0.476599000
Ti	-1.468064000	0.177473000	0.035142000
P	2.755947000	2.326779000	0.445569000
P	-1.982581000	-1.120029000	2.281786000
P	-3.117510000	2.067662000	-0.451496000
P	2.521159000	-1.159921000	-2.375381000
N	-3.234643000	-0.837290000	-0.351601000
N	3.181711000	-0.583723000	0.443540000
N	-0.210065000	0.177730000	-1.421557000
N	0.037344000	1.494897000	-0.992902000
C	-3.461098000	-2.126476000	0.175126000
C	3.884678000	1.462978000	1.602554000
C	4.357089000	-2.701622000	0.962346000
C	-3.124816000	-3.754274000	1.974499000
H	-2.680971000	-4.024083000	2.932695000
C	3.848110000	-3.606957000	-1.647560000
H	3.638796000	-3.969255000	-2.653746000
C	-4.249742000	-0.334116000	-1.191978000
C	3.639639000	-1.865905000	0.067120000
C	3.899493000	0.040483000	1.485960000
C	-2.710998000	3.388865000	-1.742150000
H	-3.655473000	3.927382000	-1.922053000
C	5.475841000	-0.049014000	3.349662000
H	6.076803000	-0.645017000	4.038750000
C	3.408982000	-2.326202000	-1.264411000
C	-2.902670000	-2.471890000	1.439721000
C	-4.412621000	1.073774000	-1.312270000
C	-3.924301000	-4.685136000	1.299265000
C	-4.816574000	-2.685188000	-1.862361000
C	-5.119302000	-1.201221000	-1.900486000
C	-4.271150000	-3.073496000	-0.504338000
C	-6.330606000	0.724669000	-2.784887000
C	3.437269000	0.715116000	-4.332461000
H	2.729913000	0.471902000	-5.135624000
H	4.313137000	1.193097000	-4.795958000
H	2.954166000	1.445569000	-3.670116000

C	1.698872000	3.513733000	1.480236000
H	0.884557000	3.770148000	0.784885000
C	4.819184000	-3.952370000	0.535505000
H	5.372782000	-4.576012000	1.239500000
C	3.872709000	3.468088000	-0.563244000
H	4.323426000	4.179890000	0.145966000
C	-6.157694000	-0.661452000	-2.669594000
H	-6.822434000	-1.339169000	-3.208002000
C	4.675467000	-0.709403000	2.411031000
C	1.380434000	-2.270132000	-3.387018000
H	2.014180000	-2.981206000	-3.941048000
C	4.558542000	-4.422764000	-0.758498000
C	-4.502243000	-4.327621000	0.072200000
H	-5.132205000	-5.042670000	-0.459621000
C	1.076466000	2.747736000	2.664271000
H	0.522041000	1.865449000	2.315226000
H	0.369441000	3.401361000	3.196878000
H	1.848643000	2.423739000	3.375399000
C	-4.577959000	-0.292222000	3.003129000
H	-4.500604000	0.285309000	2.074406000
H	-5.221505000	0.257625000	3.705708000
H	-5.067622000	-1.244950000	2.761991000
C	-5.445136000	1.583586000	-2.118600000
H	-5.558401000	2.660900000	-2.237139000
C	4.547903000	-2.217158000	2.382945000
C	-4.092040000	2.998874000	0.905596000
H	-4.747504000	2.207201000	1.297223000
C	3.037585000	4.244073000	-1.601169000
H	2.530387000	3.553608000	-2.288860000
H	3.690722000	4.902863000	-2.192737000
H	2.267006000	4.868870000	-1.129738000
C	4.695512000	2.095067000	2.563426000
H	4.708335000	3.182343000	2.622893000
C	-0.635554000	-2.014024000	3.251676000
H	-1.149383000	-2.679588000	3.962513000
C	-2.252590000	2.747431000	-3.067675000
H	-1.330157000	2.175296000	-2.916903000
H	-2.057472000	3.543007000	-3.803859000
H	-3.019509000	2.081006000	-3.481178000
C	3.878530000	-0.547056000	-3.561693000
H	4.666776000	-0.253251000	-2.850468000
C	0.547886000	-1.446090000	-4.391297000
H	-0.027443000	-0.672980000	-3.865275000
H	-0.160035000	-2.110474000	-4.909602000
H	1.172006000	-0.966909000	-5.156043000
C	4.457674000	-1.612699000	-4.509345000
H	4.837400000	-2.483116000	-3.960290000
H	5.296537000	-1.184883000	-5.079352000
H	3.707676000	-1.955165000	-5.236041000
C	5.505705000	1.350587000	3.428744000
C	2.357070000	4.823812000	1.955870000
H	3.154104000	4.636761000	2.687277000
H	1.597727000	5.445582000	2.454162000
H	2.775634000	5.415010000	1.131282000
C	0.258029000	-2.877796000	2.341135000
H	-0.324541000	-3.618387000	1.778850000
H	0.993142000	-3.417892000	2.957515000
H	0.807739000	-2.251388000	1.627985000
C	-1.660371000	4.395507000	-1.233440000
H	-1.976798000	4.906398000	-0.314464000
H	-1.490343000	5.165565000	-2.001946000
H	-0.711212000	3.879006000	-1.048353000
C	-3.195762000	-0.540740000	3.638140000
H	-2.782240000	0.425320000	3.967578000
C	0.209003000	-0.998536000	4.048045000
H	0.744688000	-0.327957000	3.364725000
H	0.954995000	-1.529330000	4.658407000
H	-0.401714000	-0.384879000	4.725336000
C	-4.990077000	4.152206000	0.420602000
H	-4.399717000	4.985360000	0.014951000
H	-5.574186000	4.545359000	1.266934000
H	-5.702015000	3.823644000	-0.346832000
C	5.006549000	2.667594000	-1.228901000
H	5.625813000	2.153389000	-0.483298000
H	5.651479000	3.345893000	-1.807550000
H	4.602117000	1.913617000	-1.916108000
C	0.448370000	-3.064335000	-2.447764000
H	1.008650000	-3.677435000	-1.730794000
H	-0.188610000	-3.732803000	-3.046645000
H	-0.206869000	-2.381351000	-1.892306000
C	-3.331791000	-1.469735000	4.858740000
H	-3.674591000	-2.469603000	4.557743000
H	-4.084344000	-1.057602000	5.548526000
H	-2.394022000	-1.575205000	5.418796000
C	-3.163052000	3.448562000	2.050594000
H	-2.519346000	2.622912000	2.381972000
H	-3.762238000	3.799168000	2.905000000
H	-2.509348000	4.275458000	1.740254000
H	0.204536000	-0.241400000	0.849303000
H	-0.534733000	1.726957000	0.227602000
H	-7.133017000	1.130649000	-3.399400000
H	-5.707443000	-3.278749000	-2.113471000
H	-4.058712000	-2.915835000	-2.636451000
H	-4.098877000	-5.672585000	1.724104000
H	4.903882000	-5.407784000	-1.069001000
H	5.422460000	-2.695699000	2.847126000
H	3.671550000	-2.515460000	2.990385000
H	6.138274000	1.850196000	4.160940000

$TS_{[H'-2]}$(open-shell singlet)

Ti	1.459893000	0.227003000	-0.486114000
Ti	-1.492349000	0.199765000	0.054368000
P	2.559533000	2.363597000	0.446435000
P	-1.915865000	-1.224716000	2.254817000
P	-3.205961000	2.032416000	-0.484345000
P	2.661646000	-1.131980000	-2.374869000
N	-3.270280000	-0.874153000	-0.316609000
N	3.181538000	-0.511614000	0.481659000
N	-0.260330000	0.049242000	-1.442510000
N	-0.034133000	1.371335000	-1.228230000
C	-3.446916000	-2.185164000	0.174789000
C	3.726414000	1.584579000	1.633200000
C	4.474519000	-2.547596000	1.038190000
C	-3.026753000	-3.858396000	1.923169000
H	-2.549265000	-4.139906000	2.861596000
C	4.069440000	-3.505222000	-1.570899000
H	3.902538000	-3.887307000	-2.577788000
C	-4.308470000	-0.395098000	-1.145343000
C	3.724356000	-1.761993000	0.121786000
C	3.840537000	0.166453000	1.529817000
C	-2.846841000	3.332539000	-1.805151000
H	-3.790958000	3.882098000	-1.950450000
C	5.384386000	0.192484000	3.421792000
H	6.009896000	-0.357629000	4.127142000
C	3.553594000	-2.245594000	-1.211969000
C	-2.851042000	-2.558044000	1.415429000
C	-4.511138000	1.007923000	-1.273382000
C	-3.816768000	-4.793392000	1.244585000
C	-4.822372000	-2.749120000	-1.848616000
C	-5.171872000	-1.277003000	-1.847580000
C	-4.242211000	-3.144134000	-0.509224000
C	-6.470235000	0.617824000	-2.678342000
C	3.576219000	0.757087000	-4.316358000
H	2.911876000	0.472129000	-5.142308000
H	4.449409000	1.263555000	-4.753844000
H	3.039309000	1.477147000	-3.685590000
C	1.455437000	3.534971000	1.462092000
H	0.600605000	3.691734000	0.786353000

C	5.015767000	-3.772396000	0.633227000
H	5.593103000	-4.355070000	1.353222000
C	3.642999000	3.544957000	-0.558977000
H	4.024372000	4.308750000	0.136255000
C	-6.248309000	-0.762867000	-2.579327000
H	-6.905914000	-1.457964000	-3.104250000
C	4.647008000	-0.524902000	2.473047000
C	1.612925000	-2.304965000	-3.415480000
H	2.297566000	-2.988692000	-3.942409000
C	4.805182000	-4.271729000	-0.659908000
C	-4.427276000	-4.417793000	0.039093000
H	-5.046719000	-5.135385000	-0.501648000
C	0.923827000	2.809759000	2.713760000
H	0.435336000	1.867088000	2.437371000
H	0.183427000	3.446487000	3.221665000
H	1.734778000	2.594583000	3.422891000
C	-4.447849000	-0.333114000	3.099511000
H	-4.380523000	0.330656000	2.230059000
H	-5.060963000	0.158383000	3.869200000
H	-4.964394000	-1.248046000	2.780605000
C	-5.582728000	1.494894000	-2.041964000
H	-5.720566000	2.569959000	-2.156338000
C	4.613663000	-2.038165000	2.456301000
C	-4.110839000	2.963585000	0.910598000
H	-4.763659000	2.180402000	1.323525000
C	2.797679000	4.227243000	-1.652871000
H	2.360071000	3.478990000	-2.327740000
H	3.425845000	4.906281000	-2.249112000
H	1.970967000	4.815682000	-1.232105000
C	4.475997000	2.273991000	2.603572000
H	4.412689000	3.359913000	2.657557000
C	-0.506123000	-2.115381000	3.125654000
H	-0.967642000	-2.844056000	3.810213000
C	-2.451426000	2.669813000	-3.141188000
H	-1.524243000	2.097681000	-3.019865000
H	-2.283646000	3.454771000	-3.894947000
H	-3.238540000	2.002470000	-3.512869000
C	4.039448000	-0.474050000	-3.508831000
H	4.782099000	-0.136143000	-2.769168000
C	0.776208000	-1.528374000	-4.453643000
H	0.137588000	-0.789070000	-3.952719000
H	0.127214000	-2.230519000	-4.998571000
H	1.401404000	-1.013373000	-5.193742000
C	4.706096000	-1.523302000	-4.416254000
H	5.103349000	-2.367636000	-3.839632000
H	5.546558000	-1.063111000	-4.957838000
H	4.003432000	-1.910136000	-5.167750000
C	5.318403000	1.591166000	3.489783000
C	2.034463000	4.914623000	1.834845000
H	2.884757000	4.830560000	2.524742000
H	1.257437000	5.501648000	2.348365000
H	2.357256000	5.492992000	0.960015000
C	0.374914000	-2.882019000	2.120785000
H	-0.205920000	-3.603954000	1.532878000
H	1.158275000	-3.432747000	2.662850000
H	0.871752000	-2.185381000	1.433145000
C	-1.758648000	4.324601000	-1.350193000
H	-2.026929000	4.848607000	-0.423039000
H	-1.608304000	5.085117000	-2.131817000
H	-0.811241000	3.793355000	-1.200365000
C	-3.056444000	-0.667772000	3.671265000
H	-2.594748000	0.261153000	4.041411000
C	0.334397000	-1.120932000	3.951758000
H	0.815197000	-0.386515000	3.293896000
H	1.124065000	-1.662748000	4.493270000
H	-0.268151000	-0.579345000	4.694459000
C	-5.009869000	4.129494000	0.458001000
H	-4.422505000	4.955037000	0.033415000
H	-5.559120000	4.527546000	1.324798000
H	-5.751536000	3.811429000	-0.285468000
C	4.847437000	2.798598000	-1.159783000
H	5.483361000	2.367876000	-0.376355000
H	5.456369000	3.492000000	-1.759621000
H	4.514940000	1.983520000	-1.815113000
C	0.686152000	-3.135242000	-2.502202000
H	1.249492000	-3.720947000	-1.764936000
H	0.098812000	-3.833388000	-3.117667000
H	-0.016577000	-2.478982000	-1.972823000
C	-3.183780000	-1.664738000	4.838147000
H	-3.584514000	-2.627054000	4.490836000
H	-3.886018000	-1.263950000	5.584867000
H	-2.228493000	-1.846272000	5.346690000
C	-3.133148000	3.399197000	2.020414000
H	-2.506670000	2.559512000	2.348784000
H	-3.695126000	3.781767000	2.886265000
H	-2.461709000	4.197958000	1.677534000
H	0.178651000	0.076655000	0.942129000
H	-0.673156000	1.775227000	0.089768000
H	-7.304137000	1.003269000	-3.263180000
H	-5.697505000	-3.366287000	-2.097878000
H	-4.070329000	-2.937424000	-2.639559000
H	-3.955349000	-5.795978000	1.646255000
H	5.211264000	-5.238819000	-0.952735000
H	5.508284000	-2.458814000	2.938149000
H	3.747967000	-2.384629000	3.053948000
H	5.901453000	2.137269000	4.230029000

$TS_{[H'-2]}$(triplet)

Ti	1.459931000	0.177657000	-0.487602000
Ti	-1.504991000	0.129028000	-0.009856000
P	2.477996000	2.398038000	0.350071000
P	-1.939349000	-1.276200000	2.182726000
P	-3.156526000	2.043681000	-0.457053000
P	2.741077000	-1.236504000	-2.295781000
N	-3.324173000	-0.865904000	-0.350037000
N	3.184462000	-0.462813000	0.533844000
N	-0.234153000	-0.215111000	-1.436227000
N	-0.110974000	1.128037000	-1.416160000
C	-3.528123000	-2.178362000	0.124252000
C	3.692871000	1.710462000	1.547012000
C	4.518953000	-2.433124000	1.214821000
C	-3.098483000	-3.892223000	1.828090000
H	-2.602400000	-4.203982000	2.747179000
C	4.174354000	-3.539155000	-1.343732000
H	4.035574000	-3.976200000	-2.332463000
C	-4.374881000	-0.332225000	-1.124310000
C	3.762149000	-1.717661000	0.248018000
C	3.832543000	0.292461000	1.534913000
C	-2.798374000	3.335361000	-1.788344000
H	-3.715581000	3.939428000	-1.878092000
C	5.384497000	0.464574000	3.412098000
H	6.020536000	-0.028220000	4.149599000
C	3.624433000	-2.274635000	-1.059913000
C	-2.907338000	-2.586170000	1.341028000
C	-4.528973000	1.079545000	-1.212135000
C	-3.930824000	-4.793599000	1.153964000
C	-4.996383000	-2.652008000	-1.855293000
C	-5.295982000	-1.168754000	-1.808725000
C	-4.375183000	-3.097748000	-0.549873000
C	-6.556619000	0.789989000	-2.542627000
C	3.674128000	0.589436000	-4.291657000
H	3.083885000	0.226475000	-5.142864000
H	4.547265000	1.120808000	-4.698510000
H	3.059218000	1.310343000	-3.737531000
C	1.352954000	3.547782000	1.375107000
H	0.457122000	3.624597000	0.741053000
C	5.092379000	-3.665732000	0.885066000
H	5.673713000	-4.194153000	1.642672000

C	3.500051000	3.597049000	-0.700385000
H	3.842784000	4.405586000	-0.036466000
C	-6.381994000	-0.600227000	-2.483319000
H	-7.086029000	-1.258443000	-2.995386000
C	4.651818000	-0.324099000	2.517981000
C	1.777372000	-2.479867000	-3.337014000
H	2.509865000	-3.141931000	-3.826065000
C	4.911071000	-4.239228000	-0.381607000
C	-4.573906000	-4.377951000	-0.021419000
H	-5.230991000	-5.068377000	-0.552990000
C	0.930454000	2.847444000	2.681696000
H	0.496851000	1.861863000	2.472022000
H	0.171442000	3.456190000	3.196060000
H	1.784972000	2.720908000	3.359760000
C	-4.445696000	-0.349951000	3.069831000
H	-4.373227000	0.328661000	2.212179000
H	-5.040820000	0.139238000	3.855007000
H	-4.984862000	-1.247537000	2.739216000
C	-5.612446000	1.620956000	-1.926346000
H	-5.715582000	2.702252000	-2.014332000
C	4.634586000	-1.835455000	2.600018000
C	-3.977579000	3.005936000	0.969465000
H	-4.654116000	2.250820000	1.396206000
C	2.621093000	4.193421000	-1.817452000
H	2.220058000	3.398285000	-2.461015000
H	3.213783000	4.878873000	-2.442088000
H	1.767210000	4.756539000	-1.417065000
C	4.439580000	2.473586000	2.463154000
H	4.357605000	3.559570000	2.447706000
C	-0.530522000	-2.193386000	3.027271000
H	-0.990707000	-2.932497000	3.701495000
C	-2.510559000	2.670347000	-3.150492000
H	-1.613732000	2.043013000	-3.081016000
H	-2.333552000	3.455112000	-3.902358000
H	-3.353100000	2.056011000	-3.490471000
C	4.145681000	-0.572734000	-3.391717000
H	4.829204000	-0.160050000	-2.633163000
C	0.940844000	-1.767857000	-4.421196000
H	0.245999000	-1.053905000	-3.960451000
H	0.350211000	-2.513916000	-4.974002000
H	1.564380000	-1.234130000	-5.149038000
C	4.908946000	-1.636053000	-4.201310000
H	5.306831000	-2.429941000	-3.557390000
H	5.759272000	-1.166601000	-4.718979000
H	4.269020000	-2.093584000	-4.969115000
C	5.299996000	1.863734000	3.384706000
C	1.866401000	4.973049000	1.661030000
H	2.759148000	4.968586000	2.300723000
H	1.085943000	5.533335000	2.198789000
H	2.100861000	5.533191000	0.747057000
C	0.336641000	-2.945536000	1.999783000
H	-0.252309000	-3.661239000	1.412289000
H	1.132077000	-3.499382000	2.520466000
H	0.818379000	-2.239137000	1.310863000
C	-1.632024000	4.256682000	-1.384241000
H	-1.817367000	4.782044000	-0.437567000
H	-1.477974000	5.018097000	-2.164241000
H	-0.710505000	3.669637000	-1.291300000
C	-3.056137000	-0.724627000	3.620869000
H	-2.571658000	0.187143000	4.004508000
C	0.322134000	-1.219696000	3.865681000
H	0.802337000	-0.475428000	3.218219000
H	1.112246000	-1.776342000	4.391398000
H	-0.271979000	-0.688945000	4.622777000
C	-4.831101000	4.219753000	0.557068000
H	-4.216596000	5.020022000	0.122425000
H	-5.332099000	4.634791000	1.444908000
H	-5.611047000	3.948391000	-0.165384000
C	4.740663000	2.892226000	-1.277402000
H	5.399741000	2.524391000	-0.481240000
H	5.311336000	3.593660000	-1.904949000
H	4.450355000	2.037691000	-1.901725000
C	0.858140000	-3.333270000	-2.437295000
H	1.421370000	-3.880430000	-1.671145000
H	0.323011000	-4.067290000	-3.058647000
H	0.111921000	-2.698818000	-1.942907000
C	-3.192819000	-1.742490000	4.768415000
H	-3.616080000	-2.689064000	4.404890000
H	-3.879630000	-1.343698000	5.530437000
H	-2.236561000	-1.953993000	5.263503000
C	-2.945942000	3.382686000	2.051246000
H	-2.347062000	2.511952000	2.348539000
H	-3.460860000	3.778064000	2.940274000
H	-2.251926000	4.156366000	1.695554000
H	0.145398000	0.101169000	0.920802000
H	-0.581403000	1.650447000	0.003040000
H	-7.399471000	1.218207000	-3.083217000
H	-5.901412000	-3.234014000	-2.081294000
H	-4.284312000	-2.846200000	-2.680932000
H	-4.080655000	-5.801166000	1.538905000
H	5.342953000	-5.211053000	-0.616021000
H	5.527084000	-2.214806000	3.118399000
H	3.763980000	-2.151682000	3.207212000
H	5.880788000	2.466712000	4.081304000

$TS_{[H'-3]}$(closed-shell singlet)

Ti	-1.357724000	-0.507727000	0.099367000
Ti	1.345337000	-0.037800000	-0.084912000
P	-2.223994000	0.714323000	2.289379000
P	1.961939000	2.371489000	-0.928524000
P	2.989413000	-0.951734000	1.884216000
P	-2.744757000	-2.403759000	-1.090200000
N	3.216880000	-0.285184000	-1.005252000
N	-3.262712000	0.468786000	-0.470218000
N	0.111917000	-0.913710000	-1.073065000
N	0.032687000	-1.401905000	0.808292000
C	3.573123000	0.471391000	-2.137251000
C	-3.330029000	1.938660000	1.498486000
C	-4.884833000	0.885423000	-2.297637000
C	3.441241000	2.573135000	-3.388458000
H	3.038743000	3.579021000	-3.504097000
C	-4.741597000	-1.812205000	-3.045795000
H	-4.653137000	-2.850027000	-3.366610000
C	4.105548000	-1.309838000	-0.638103000
C	-4.021192000	0.019293000	-1.568533000
C	-3.703683000	1.653709000	0.146527000
C	2.491287000	-2.347206000	3.054806000
H	3.398500000	-2.630123000	3.611746000
C	-5.050576000	3.700361000	0.162830000
H	-5.709345000	4.387062000	-0.371942000
C	-3.950077000	-1.349517000	-1.977812000
C	3.073627000	1.798615000	-2.274240000
C	4.154502000	-1.757909000	0.715421000
C	4.318044000	2.069456000	-4.358195000
C	4.844805000	-1.495515000	-3.033599000
C	4.991865000	-1.899087000	-1.582662000
C	4.435379000	-0.042756000	-3.139059000
C	5.958649000	-3.310822000	0.160111000
C	-3.000829000	-4.242088000	1.083427000
H	-2.312621000	-5.010174000	0.707861000
H	-3.686714000	-4.728670000	1.793042000
H	-2.402036000	-3.501288000	1.627919000
C	-1.024700000	1.621121000	3.450383000
H	-0.235298000	0.867637000	3.596370000
C	-5.688387000	0.384153000	-3.326048000
H	-6.350059000	1.072626000	-3.854909000
C	-3.371052000	-0.209286000	3.480312000
H	-3.714029000	0.534748000	4.215975000

C	5.912771000	-2.865776000	-1.169574000
H	6.589036000	-3.296439000	-1.910091000
C	-4.552200000	2.585120000	-0.517216000
C	-1.920232000	-3.442028000	-2.431271000
H	-2.697845000	-4.106403000	-2.841245000
C	-5.630867000	-0.962547000	-3.711538000
C	4.810249000	0.764469000	-4.219358000
H	5.477465000	0.351251000	-4.977795000
C	-0.381905000	2.835673000	2.753040000
H	0.082552000	2.544583000	1.804128000
H	0.392973000	3.263663000	3.407023000
H	-1.124366000	3.617343000	2.546586000
C	4.371582000	3.123394000	0.317887000
H	4.285610000	2.128701000	0.770895000
H	4.900859000	3.782029000	1.022800000
H	4.985978000	3.022834000	-0.586619000
C	5.067226000	-2.762766000	1.088352000
H	5.082626000	-3.119857000	2.117909000
C	-4.829658000	2.363681000	-1.986176000
C	4.131352000	0.177067000	2.911886000
H	4.779308000	0.607346000	2.133915000
C	-2.615097000	-1.337165000	4.209705000
H	-2.235526000	-2.078869000	3.494624000
H	-3.291744000	-1.852288000	4.907995000
H	-1.758741000	-0.964117000	4.786686000
C	-3.839281000	3.077642000	2.149219000
H	-3.564466000	3.269746000	3.184840000
C	0.646276000	3.395002000	-1.817139000
H	1.205506000	4.176615000	-2.355010000
C	1.970394000	-3.584379000	2.294253000
H	1.087973000	-3.315502000	1.701336000
H	1.693135000	-4.361017000	3.024385000
H	2.730878000	-4.002182000	1.623597000
C	-3.808356000	-3.596485000	-0.062978000
H	-4.545479000	-2.910211000	0.380960000
C	-0.787551000	-4.298909000	-1.827028000
H	-0.048171000	-3.658214000	-1.330185000
H	-0.282525000	-4.854677000	-2.631279000
H	-1.160452000	-5.032118000	-1.100351000
C	-4.578663000	-4.656880000	-0.871032000
H	-5.208843000	-4.202834000	-1.645580000
H	-5.236318000	-5.225905000	-0.196580000
H	-3.896916000	-5.374624000	-1.347838000
C	-4.706831000	3.959697000	1.496936000
C	-1.558768000	2.019138000	4.843471000
H	-2.344318000	2.783417000	4.783688000
H	-0.731464000	2.448360000	5.428714000
H	-1.954156000	1.167745000	5.410206000
C	-0.156328000	2.588108000	-2.853772000
H	0.498430000	2.067776000	-3.563895000
H	-0.804732000	3.275863000	-3.419673000
H	-0.794650000	1.842646000	-2.363504000
C	1.429308000	-1.850942000	4.056179000
H	1.786512000	-1.011513000	4.668422000
H	1.153041000	-2.667744000	4.740229000
H	0.528872000	-1.537322000	3.512807000
C	2.990811000	3.713164000	-0.031393000
H	2.438151000	3.889571000	0.905865000
C	-0.302944000	4.075553000	-0.810583000
H	-0.903943000	3.325901000	-0.281753000
H	-0.992918000	4.743831000	-1.347170000
H	0.232145000	4.678455000	-0.063787000
C	5.035533000	-0.536450000	3.932897000
H	4.452826000	-0.975918000	4.754501000
H	5.733911000	0.189282000	4.376696000
H	5.633293000	-1.328612000	3.464725000
C	-4.608246000	-0.754087000	2.743817000
H	-5.171496000	0.047862000	2.252050000
H	-5.273778000	-1.257128000	3.461447000
H	-4.321004000	-1.486072000	1.978827000
C	-1.375919000	-2.557751000	-3.572363000
H	-2.165979000	-1.957628000	-4.040243000
H	-0.933467000	-3.205609000	-4.344277000
H	-0.596379000	-1.885135000	-3.194964000
C	3.164734000	5.059639000	-0.759697000
H	3.684863000	4.925374000	-1.717970000
H	3.781456000	5.732010000	-0.143021000
H	2.211083000	5.568403000	-0.948686000
C	3.344040000	1.330956000	3.566250000
H	2.713519000	1.852334000	2.834356000
H	4.040754000	2.062608000	4.002558000
H	2.694680000	0.970128000	4.375783000
H	0.803850000	0.390982000	-1.716407000
H	-0.213192000	1.000731000	0.282560000
H	6.669599000	-4.078086000	0.462960000
H	5.771866000	-1.688447000	-3.592586000
H	4.060947000	-2.122202000	-3.501697000
H	4.603352000	2.679742000	-5.213908000
H	-4.015903000	2.824732000	-2.580267000
H	-5.757855000	2.867423000	-2.293186000
H	-6.247531000	-1.334006000	-4.528440000
H	-5.100064000	4.834129000	2.013098000

2m^{L1}(closed-shell singlet)

Ti	1.321677000	0.119867000	-0.177259000
Ti	-1.337642000	0.379923000	-0.505767000
N	0.336054000	0.676509000	-1.635325000
N	-0.775526000	1.148815000	-2.119211000
N	-3.112346000	-0.465268000	0.415901000
N	3.288958000	-0.370645000	-0.600342000
P	-1.871874000	-1.886583000	-1.662399000
P	-2.792891000	2.441808000	0.340320000
P	2.620042000	2.379554000	-0.233029000
P	2.116530000	-1.468894000	1.752058000
H	0.011967000	1.087863000	0.768853000
H	-0.157011000	-0.857482000	0.299624000
C	-2.381088000	-2.729657000	-0.111228000
C	-2.991270000	-1.822418000	0.802709000
C	-3.379665000	-2.302589000	2.074384000
H	-3.845400000	-1.615573000	2.779554000
C	-3.153266000	-3.635491000	2.434442000
H	-3.455856000	-3.981297000	3.423181000
C	-2.524679000	-4.519231000	1.544040000
C	-2.140305000	-4.058494000	0.275454000
H	-1.647760000	-4.745237000	-0.409684000
C	-3.357748000	-1.928537000	-2.853791000
H	-2.893526000	-2.179731000	-3.820911000
C	-4.401339000	-3.007940000	-2.512553000
H	-4.887936000	-2.789114000	-1.553260000
H	-3.959600000	-4.010157000	-2.444708000
H	-5.179771000	-3.028776000	-3.290715000
C	-4.008485000	-0.539092000	-2.998172000
H	-4.752703000	-0.561251000	-3.809571000
H	-3.259154000	0.226185000	-3.236662000
H	-4.524789000	-0.244850000	-2.075856000
C	-0.600485000	-2.960771000	-2.540347000
H	0.151274000	-3.178265000	-1.768185000
C	-1.113101000	-4.288666000	-3.138997000
H	-1.810065000	-4.107888000	-3.969161000
H	-1.620904000	-4.931846000	-2.410721000
H	-0.259426000	-4.850932000	-3.546664000
C	0.072551000	-2.115258000	-3.645538000
H	0.870626000	-2.704018000	-4.120967000
H	0.508478000	-1.196550000	-3.236967000
H	-0.648366000	-1.838130000	-4.429225000
C	-4.336938000	0.176993000	0.636890000
C	-4.397417000	1.606413000	0.601055000
C	-5.628185000	2.272973000	0.740912000

H	-5.654526000	3.361590000	0.690867000
C	-6.822967000	1.568839000	0.931879000
C	-6.772109000	0.166608000	0.974363000
H	-7.690026000	-0.406881000	1.107300000
C	-5.564270000	-0.517877000	0.828363000
H	-5.561660000	-1.605902000	0.844886000
C	-2.373931000	3.248061000	1.997634000
H	-1.409347000	3.743745000	1.814295000
C	-2.155493000	2.146148000	3.053227000
H	-1.838981000	2.598679000	4.005131000
H	-1.382525000	1.437838000	2.729867000
H	-3.085243000	1.589321000	3.234593000
C	-3.390318000	4.295334000	2.487057000
H	-4.368592000	3.834687000	2.678164000
H	-3.526499000	5.116660000	1.770468000
H	-3.037714000	4.734636000	3.432543000
C	-3.177264000	3.874859000	-0.817295000
H	-4.000309000	4.452179000	-0.367328000
C	-3.636091000	3.336851000	-2.187603000
H	-3.890506000	4.179641000	-2.847981000
H	-4.523469000	2.697870000	-2.093663000
H	-2.832635000	2.758106000	-2.661205000
C	-1.951546000	4.795473000	-0.973777000
H	-1.107370000	4.236917000	-1.398297000
H	-1.634997000	5.237788000	-0.019367000
H	-2.193040000	5.619669000	-1.661281000
C	4.316218000	1.796990000	-0.641791000
C	4.431131000	0.383272000	-0.822406000
C	5.708023000	-0.156568000	-1.125381000
H	5.822503000	-1.232842000	-1.243559000
C	6.820756000	0.679989000	-1.246659000
H	7.790977000	0.238799000	-1.476883000
C	6.710137000	2.067319000	-1.064271000
C	5.454841000	2.611078000	-0.755055000
H	5.365821000	3.685085000	-0.591382000
C	2.138934000	3.524049000	-1.669359000
H	1.046520000	3.605090000	-1.573183000
C	2.441683000	2.828183000	-3.013036000
H	2.014917000	3.422074000	-3.834920000
H	2.001485000	1.825757000	-3.050551000
H	3.525487000	2.747595000	-3.173505000
C	2.752958000	4.937128000	-1.647105000
H	3.846233000	4.899305000	-1.748921000
H	2.509384000	5.497967000	-0.735580000
H	2.366004000	5.511965000	-2.502311000
C	2.887146000	3.533676000	1.235500000
H	3.568720000	4.335820000	0.912414000
C	1.546652000	4.148619000	1.679532000
H	0.855050000	3.352318000	1.985565000
H	1.066334000	4.727715000	0.879075000
H	1.703926000	4.821436000	2.536123000
C	3.538789000	2.765914000	2.399297000
H	3.682950000	3.437218000	3.259495000
H	4.515018000	2.352474000	2.116372000
H	2.890811000	1.937435000	2.716092000
C	3.169076000	-1.751494000	-0.801585000
C	2.502836000	-2.478341000	0.241407000
C	2.204935000	-3.844063000	0.043128000
H	1.674079000	-4.400346000	0.813040000
C	2.609119000	-4.505876000	-1.120970000
C	3.300873000	-3.799350000	-2.123586000
H	3.617558000	-4.314788000	-3.030257000
C	3.561144000	-2.436764000	-1.980739000
H	4.052869000	-1.878761000	-2.775674000
C	3.792042000	-1.386076000	2.647748000
H	4.321491000	-0.645090000	2.029685000
C	4.631397000	-2.678204000	2.657992000
H	5.638883000	-2.454761000	3.041578000
H	4.739656000	-3.099380000	1.650991000
H	4.192104000	-3.446161000	3.306954000
C	3.640217000	-0.799478000	4.066931000
H	3.176066000	-1.520463000	4.753094000
H	3.034000000	0.115316000	4.072907000
H	4.631919000	-0.549466000	4.471967000
C	0.891701000	-2.502854000	2.745736000
H	0.200398000	-2.857190000	1.966117000
C	1.422343000	-3.719111000	3.532176000
H	2.034387000	-3.407621000	4.389095000
H	2.026240000	-4.398576000	2.918360000
H	0.569650000	-4.290826000	3.928698000
C	0.084436000	-1.562704000	3.669264000
H	-0.727577000	-2.125769000	4.151117000
H	-0.359752000	-0.742794000	3.093182000
H	0.714783000	-1.133761000	4.460952000
H	-7.768468000	2.098472000	1.035624000
H	-2.339945000	-5.554226000	1.829182000
H	2.396135000	-5.566826000	-1.246056000
H	7.583040000	2.711596000	-1.155937000

TS_{IJ}^{L1} (clodes-shell singlet)

Ti	1.674127000	0.184615000	0.400386000
Ti	-1.903849000	-0.038769000	-0.154719000
N	-0.110703000	-0.576440000	-0.010671000
N	-0.137128000	0.787381000	-0.230959000
N	-3.585290000	-0.512962000	0.840304000
N	3.123511000	-0.444987000	-0.917780000
P	-2.907297000	-1.645356000	-1.792947000
P	-3.006528000	2.232994000	0.385633000
P	2.708979000	2.338786000	-0.527866000
P	3.423945000	-1.182766000	1.796864000
H	1.416072000	1.124251000	1.873006000
H	1.114899000	-0.004376000	2.045132000
C	-2.992564000	-2.614118000	-0.215072000
C	-3.390766000	-1.901335000	0.970468000
C	-3.430621000	-2.589517000	2.210484000
H	-3.719029000	-2.039409000	3.104678000
C	-3.076008000	-3.933887000	2.289300000
H	-3.115536000	-4.445781000	3.250516000
C	-2.636345000	-4.623405000	1.141874000
C	-2.585104000	-3.963383000	-0.085765000
H	-2.244736000	-4.508210000	-0.963913000
C	-4.596452000	-1.823253000	-2.658352000
H	-4.349311000	-1.771257000	-3.732008000
C	-5.313417000	-3.154166000	-2.363466000
H	-5.559382000	-3.231206000	-1.296164000
H	-4.711512000	-4.029470000	-2.634383000
H	-6.254500000	-3.201018000	-2.932386000
C	-5.499985000	-0.625634000	-2.310233000
H	-6.437500000	-0.685894000	-2.883770000
H	-5.009690000	0.326433000	-2.543184000
H	-5.754202000	-0.618407000	-1.242236000
C	-1.665455000	-2.543247000	-2.901977000
H	-0.880846000	-2.863389000	-2.201341000
C	-2.167740000	-3.762201000	-3.701623000
H	-2.956620000	-3.481783000	-4.413363000
H	-2.557965000	-4.564021000	-3.062882000
H	-1.333332000	-4.178705000	-4.285910000
C	-1.047962000	-1.495465000	-3.856516000
H	-0.270960000	-1.966558000	-4.477178000
H	-0.589860000	-0.670888000	-3.297478000
H	-1.805103000	-1.073951000	-4.534832000
C	-4.624840000	0.233709000	1.392705000
C	-4.541479000	1.651682000	1.229926000
C	-5.586640000	2.463299000	1.695468000
H	-5.532717000	3.543009000	1.556075000
C	-6.713125000	1.908736000	2.325216000
C	-6.790438000	0.518394000	2.481897000
H	-7.662691000	0.072687000	2.960432000

C	-5.764827000	-0.317060000	2.022108000
H	-5.851014000	-1.397001000	2.130517000
C	-2.007047000	3.065159000	1.768463000
H	-1.048521000	3.304386000	1.282826000
C	-1.721148000	2.029169000	2.875455000
H	-1.084541000	2.481428000	3.650441000
H	-1.186040000	1.153993000	2.484111000
H	-2.652911000	1.693991000	3.352484000
C	-2.618274000	4.345339000	2.365885000
H	-3.580020000	4.133124000	2.853162000
H	-2.776110000	5.131200000	1.615129000
H	-1.941970000	4.752907000	3.132867000
C	-3.576537000	3.682265000	-0.685834000
H	-4.106892000	4.395111000	-0.035357000
C	-4.545094000	3.197555000	-1.779375000
H	-4.888944000	4.051965000	-2.381791000
H	-5.425308000	2.701857000	-1.350839000
H	-4.041780000	2.487598000	-2.450379000
C	-2.357424000	4.388204000	-1.311329000
H	-1.778858000	3.685454000	-1.927108000
H	-1.685370000	4.809946000	-0.551966000
H	-2.692464000	5.212667000	-1.958410000
C	4.111719000	1.660969000	-1.511404000
C	4.101080000	0.233693000	-1.629222000
C	5.117040000	-0.391073000	-2.396549000
H	5.131807000	-1.476832000	-2.482010000
C	6.106531000	0.376122000	-3.018710000
H	6.879915000	-0.127717000	-3.599421000
C	6.126676000	1.774242000	-2.894482000
C	5.127182000	2.402592000	-2.135915000
H	5.148064000	3.486710000	-2.021105000
C	1.641595000	3.237720000	-1.813207000
H	0.712995000	3.458749000	-1.266675000
C	1.296570000	2.269568000	-2.962548000
H	0.583419000	2.750039000	-3.650150000
H	0.837462000	1.351776000	-2.577847000
H	2.196818000	2.006070000	-3.534705000
C	2.230782000	4.546914000	-2.370515000
H	3.164698000	4.358245000	-2.917559000
H	2.431067000	5.291555000	-1.589083000
H	1.518962000	4.995448000	-3.080713000
C	3.452151000	3.725590000	0.508590000
H	3.958176000	4.433266000	-0.166398000
C	2.330965000	4.458451000	1.272023000
H	1.782888000	3.747661000	1.906771000
H	1.611217000	4.939664000	0.595221000
H	2.761523000	5.239916000	1.916190000
C	4.485203000	3.144305000	1.490632000
H	4.905727000	3.946853000	2.115709000
H	5.310657000	2.649975000	0.962181000
H	4.004124000	2.407201000	2.149155000
C	2.962586000	-1.837824000	-0.843559000
C	2.910757000	-2.384439000	0.481052000
C	2.509374000	-3.725182000	0.656293000
H	2.426892000	-4.142380000	1.658431000
C	2.234170000	-4.538895000	-0.447281000
C	2.355908000	-4.017190000	-1.749705000
H	2.158400000	-4.657648000	-2.609798000
C	2.700998000	-2.680305000	-1.952216000
H	2.741502000	-2.260646000	-2.956477000
C	5.322473000	-1.181600000	1.625211000
H	5.440687000	-0.604540000	0.695061000
C	6.008644000	-2.545830000	1.420775000
H	7.056531000	-2.385877000	1.122845000
H	5.519975000	-3.131594000	0.632154000
H	6.013920000	-3.143996000	2.340489000
C	5.982312000	-0.375413000	2.763066000
H	5.938583000	-0.915140000	3.719157000
H	5.505082000	0.603377000	2.899739000
H	7.043897000	-0.204183000	2.530214000
C	2.918856000	-1.979800000	3.433934000
H	1.912281000	-2.358783000	3.198024000
C	3.777080000	-3.141643000	3.974300000
H	4.766634000	-2.791251000	4.296530000
H	3.926279000	-3.939882000	3.237089000
H	3.283771000	-3.581542000	4.854888000
C	2.754418000	-0.877563000	4.504974000
H	2.319108000	-1.307986000	5.419658000
H	2.093126000	-0.078698000	4.148298000
H	3.722188000	-0.432409000	4.774735000
H	-7.516511000	2.552474000	2.679992000
H	-2.343997000	-5.670397000	1.209593000
H	1.940147000	-5.577159000	-0.298594000
H	6.907259000	2.363086000	-3.373755000

2m^{L2}(closed-shell singlet)

Ti	1.273531000	0.416156000	-0.586291000
Ti	-1.246834000	0.621556000	0.384069000
P	2.681902000	2.536359000	0.307117000
P	-1.291540000	-0.986211000	2.633603000
P	-3.424690000	2.015919000	-0.652084000
P	1.652773000	-1.833133000	-2.020600000
N	-2.820905000	-0.709978000	0.182557000
N	3.240689000	-0.273490000	-0.156151000
N	-0.515966000	1.239628000	-1.167927000
N	0.518368000	1.377440000	-1.968421000
C	-2.906973000	-1.982887000	0.724882000
C	4.148352000	1.705822000	1.027340000
C	4.953858000	-1.792084000	0.351069000
C	-2.394325000	-3.725313000	2.284322000
H	-1.869493000	-4.113651000	3.157168000
C	3.706573000	-3.804115000	-1.198929000
H	3.261680000	-4.600991000	-1.794917000
C	-3.837317000	-0.649742000	-0.757283000
C	3.723290000	-1.563470000	-0.340289000
C	4.195782000	0.351659000	0.634936000
C	-3.215203000	3.262872000	-2.054276000
H	-4.215709000	3.670275000	-2.267918000
C	6.309071000	-0.021023000	1.789940000
H	7.143084000	-0.655320000	2.090869000
C	3.097292000	-2.539939000	-1.139443000
C	-2.197359000	-2.397606000	1.867483000
C	-4.256774000	0.539458000	-1.382849000
C	-3.283945000	-4.575675000	1.585087000
C	-4.495492000	-1.909298000	-0.925171000
C	-3.876967000	-2.792769000	0.055260000
C	-5.917452000	-0.827306000	-2.559463000
C	1.512908000	-0.556816000	-4.608315000
H	0.715353000	-1.161441000	-5.060962000
H	2.110105000	-0.136647000	-5.431811000
H	1.052997000	0.268743000	-4.050787000
C	1.999362000	3.782341000	1.551392000
H	1.037308000	4.078830000	1.102850000
C	5.536387000	-3.070043000	0.270802000
H	6.467726000	-3.294893000	0.790897000
C	3.377975000	3.595725000	-1.093036000
H	4.128568000	4.267309000	-0.647633000
C	-5.539294000	-1.986358000	-1.864303000
H	-6.065600000	-2.923769000	-2.045275000
C	5.270302000	-0.526264000	0.988865000
C	0.418530000	-3.221890000	-2.303202000
H	0.887981000	-3.931771000	-3.002498000
C	4.903454000	-4.062640000	-0.490597000
C	-4.039869000	-4.119617000	0.493874000
H	-4.751147000	-4.788795000	0.009216000
C	1.703852000	3.088633000	2.895943000
H	1.048277000	2.220866000	2.754882000
H	1.207729000	3.795797000	3.577768000

H	2.631556000	2.747065000	3.374807000
C	-3.750961000	0.043394000	3.555024000
H	-3.589904000	0.863279000	2.841580000
H	-4.364617000	0.425813000	4.384526000
H	-4.321668000	-0.742038000	3.041491000
C	-5.309434000	0.425151000	-2.308249000
H	-5.675920000	1.303900000	-2.838770000
C	-4.808760000	2.712012000	0.457724000
H	-5.110599000	1.810515000	1.014333000
C	2.256062000	4.422477000	-1.752460000
H	1.483911000	3.754642000	-2.157928000
H	2.672277000	5.015509000	-2.580670000
H	1.780594000	5.120300000	-1.049254000
C	5.214195000	2.179944000	1.811896000
H	5.245446000	3.220401000	2.130616000
C	0.194288000	-1.754156000	3.501476000
H	-0.205764000	-2.553012000	4.146096000
C	-2.670529000	2.607801000	-3.341140000
H	-1.666974000	2.198359000	-3.181098000
H	-2.610474000	3.371953000	-4.131553000
H	-3.320964000	1.799253000	-3.695361000
C	2.425887000	-1.415923000	-3.709373000
H	3.279387000	-0.791625000	-3.398250000
C	-0.882804000	-2.675341000	-2.929485000
H	-1.330772000	-1.906779000	-2.286700000
H	-1.608882000	-3.494520000	-3.035014000
H	-0.720240000	-2.239576000	-3.922127000
C	2.976033000	-2.637862000	-4.468313000
H	3.668304000	-3.225675000	-3.852793000
H	3.521909000	-2.299207000	-5.361811000
H	2.164114000	-3.294995000	-4.811188000
C	6.269610000	1.321135000	2.194058000
C	2.844976000	5.055060000	1.764326000
H	3.807610000	4.823627000	2.237827000
H	2.304952000	5.739425000	2.435954000
H	3.042814000	5.594446000	0.830022000
C	1.175491000	-2.387081000	2.498624000
H	0.689078000	-3.157785000	1.889717000
H	2.008090000	-2.855336000	3.045131000
H	1.591212000	-1.629933000	1.822886000
C	-2.290453000	4.415896000	-1.608039000
H	-2.682045000	4.957166000	-0.736677000
H	-2.177718000	5.140631000	-2.428299000
H	-1.295218000	4.026505000	-1.357196000
C	-2.415591000	-0.506546000	4.093770000
H	-1.875713000	0.325972000	4.574570000
C	0.912254000	-0.719180000	4.390750000
H	1.306402000	0.105748000	3.783761000
H	1.762266000	-1.196907000	4.899744000
H	0.254838000	-0.298471000	5.163999000
C	-6.049389000	3.262805000	-0.267175000
H	-5.818276000	4.182252000	-0.823428000
H	-6.830567000	3.512301000	0.467102000
H	-6.469549000	2.527593000	-0.964570000
C	4.075175000	2.697957000	-2.134881000
H	4.869026000	2.088994000	-1.684288000
H	4.525642000	3.326001000	-2.918079000
H	3.348928000	2.028687000	-2.615526000
C	0.109783000	-3.951862000	-0.981488000
H	1.011382000	-4.378263000	-0.524828000
H	-0.602036000	-4.768006000	-1.173341000
H	-0.353566000	-3.265541000	-0.262963000
C	-2.660089000	-1.610886000	5.137333000
H	-3.152682000	-2.479009000	4.678758000
H	-3.319270000	-1.232699000	5.933771000
H	-1.730359000	-1.950529000	5.612561000
C	-4.256826000	3.731078000	1.477232000
H	-3.364020000	3.349117000	1.992618000
H	-5.019288000	3.952402000	2.238828000
H	-3.988473000	4.681010000	0.995239000
H	-0.011083000	-0.757985000	0.175457000
H	0.444937000	0.889747000	1.089344000
H	-6.723529000	-0.883315000	-3.290391000
H	-3.406567000	-5.603447000	1.925533000
H	5.348107000	-5.055395000	-0.551040000
H	7.076190000	1.718853000	2.809055000

$TS_{H'I}^{L2}$ (closed-shell singlet)

Ti	-1.584903000	-0.353468000	0.046895000
Ti	1.640904000	0.374878000	0.355715000
P	-2.346753000	1.231142000	2.155836000
P	2.016731000	2.510075000	-1.205540000
P	2.906182000	-1.622768000	1.761556000
P	-2.564439000	-2.196749000	-1.605321000
N	3.591574000	0.204238000	-0.465281000
N	-3.655818000	0.130142000	-0.218506000
N	-0.034943000	0.000439000	-0.825683000
N	0.162218000	-0.958563000	0.250565000
C	4.183413000	0.986594000	-1.461764000
C	-4.012845000	1.767436000	1.604279000
C	-5.729876000	0.346859000	-1.289141000
C	4.344065000	2.820506000	-3.008821000
H	3.944186000	3.727429000	-3.462320000
C	-5.072296000	-1.730185000	-3.097516000
H	-4.859706000	-2.529852000	-3.807071000
C	4.509890000	-0.829254000	-0.258330000
C	-4.473258000	-0.334559000	-1.238961000
C	-4.418771000	1.085107000	0.439263000
C	2.281267000	-3.392393000	1.983785000
H	3.095848000	-3.968946000	2.450527000
C	-6.577710000	2.214255000	0.396824000
H	-7.558672000	2.400734000	-0.040451000
C	-4.140490000	-1.398782000	-2.099239000
C	3.627650000	2.162692000	-1.994841000
C	4.385073000	-1.848529000	0.703443000
C	5.578866000	2.309657000	-3.468151000
C	5.644639000	-0.738536000	-1.126219000
C	5.433174000	0.460626000	-1.910514000
C	6.491070000	-2.780970000	-0.144052000
C	-2.109258000	-4.413582000	0.156798000
H	-1.284821000	-4.863182000	-0.411316000
H	-2.566816000	-5.207893000	0.765184000
H	-1.675481000	-3.667027000	0.834654000
C	-1.396753000	2.739270000	2.758830000
H	-0.361375000	2.370326000	2.815952000
C	-6.641547000	-0.013337000	-2.297527000
H	-7.607096000	0.485039000	-2.384425000
C	-2.675582000	0.183820000	3.691031000
H	-3.231048000	0.814428000	4.402238000
C	6.636303000	-1.732051000	-1.060861000
H	7.506765000	-1.694569000	-1.716151000
C	-5.698798000	1.277163000	-0.173723000
C	-1.704782000	-2.691210000	-3.202742000
H	-2.355507000	-3.430164000	-3.696325000
C	-6.298090000	-1.032349000	-3.198113000
C	6.127530000	1.138654000	-2.928045000
H	7.080110000	0.760876000	-3.300198000
C	-1.444810000	3.832852000	1.674370000
H	-1.074701000	3.446637000	0.718010000
H	-0.803724000	4.674862000	1.974466000
H	-2.465827000	4.211761000	1.531038000
C	3.264364000	3.739914000	0.961898000
H	2.896789000	2.892027000	1.557502000
H	3.375201000	4.610216000	1.626830000
H	4.258460000	3.484806000	0.568721000
C	5.385057000	-2.836670000	0.732336000
H	5.312858000	-3.666472000	1.435342000
C	3.684101000	-1.108829000	3.420299000

H	4.290098000	-0.245450000	3.101349000
C	-1.349086000	-0.272701000	4.328619000
H	-0.744296000	-0.843244000	3.611604000
H	-1.554928000	-0.918888000	5.195037000
H	-0.738631000	0.570820000	4.674179000
C	-4.928165000	2.678446000	2.159916000
H	-4.682238000	3.221529000	3.070752000
C	0.916080000	3.036728000	-2.638659000
H	1.409778000	3.899766000	-3.113551000
C	1.971520000	-4.002799000	0.601249000
H	1.192085000	-3.420199000	0.094136000
H	1.611469000	-5.036030000	0.726061000
H	2.860968000	-4.024988000	-0.040423000
C	-3.172875000	-3.792949000	-0.770798000
H	-3.989021000	-3.406177000	-0.139462000
C	-0.328489000	-3.329161000	-2.924692000
H	0.315125000	-2.633860000	-2.370822000
H	0.164682000	-3.567721000	-3.878473000
H	-0.409070000	-4.260285000	-2.349659000
C	-3.763939000	-4.836061000	-1.736307000
H	-4.553103000	-4.406196000	-2.365928000
H	-4.207483000	-5.663001000	-1.161863000
H	-2.989388000	-5.265501000	-2.386994000
C	-6.184857000	2.903085000	1.553238000
C	-1.823271000	3.298832000	4.130764000
H	-2.838729000	3.715489000	4.103817000
H	-1.140977000	4.115847000	4.409113000
H	-1.781531000	2.548621000	4.930150000
C	0.826201000	1.894171000	-3.669002000
H	1.813400000	1.641619000	-4.076064000
H	0.175275000	2.195859000	-4.503669000
H	0.404936000	0.995258000	-3.203225000
C	1.040684000	-3.462944000	2.895064000
H	1.253690000	-3.131165000	3.918571000
H	0.677225000	-4.500708000	2.948759000
H	0.232123000	-2.840050000	2.491193000
C	2.287442000	4.073828000	-0.185110000
H	1.299285000	4.270340000	0.257869000
C	-0.481263000	3.469612000	-2.157266000
H	-0.985241000	2.644508000	-1.636987000
H	-1.100193000	3.756805000	-3.020524000
H	-0.436437000	4.331246000	-1.477641000
C	4.618999000	-2.152062000	4.058309000
H	4.064111000	-3.043701000	4.384859000
H	5.098263000	-1.721019000	4.950630000
H	5.413575000	-2.466047000	3.371101000
C	-3.557072000	-1.024920000	3.318020000
H	-4.500143000	-0.714953000	2.851205000
H	-3.791840000	-1.608648000	4.220391000
H	-3.033915000	-1.695670000	2.618350000
C	-1.561611000	-1.463094000	-4.123687000
H	-2.533877000	-1.015793000	-4.364696000
H	-1.077324000	-1.766575000	-5.063589000
H	-0.935121000	-0.698583000	-3.648969000
C	2.747263000	5.310262000	-0.976924000
H	3.724730000	5.134388000	-1.446245000
H	2.853547000	6.168747000	-0.296107000
H	2.032460000	5.596302000	-1.760665000
C	2.650133000	-0.591644000	4.440776000
H	1.971988000	0.132381000	3.973399000
H	3.175119000	-0.096824000	5.272181000
H	2.056516000	-1.410217000	4.870544000
H	1.718388000	0.829028000	2.029929000
H	7.247840000	-3.563349000	-0.095371000
H	6.110266000	2.836413000	-4.260207000
H	-6.998241000	-1.307884000	-3.985826000
H	-6.865878000	3.623987000	2.003991000
H	0.710446000	1.737625000	0.853876000

TS_{IJ}^{L2} (closed-shell singlet)

Ti	1.657811000	0.335694000	-0.565698000
Ti	-1.669871000	0.926700000	0.643977000
P	3.194289000	2.307188000	0.330929000
P	-2.027205000	-0.505767000	2.854071000
P	-3.072622000	1.986011000	-1.322695000
P	1.698404000	-1.992984000	-1.865015000
N	-3.228661000	-0.414987000	0.246732000
N	3.528807000	-0.552033000	-0.140482000
N	0.240604000	0.289720000	0.599516000
N	-0.120902000	1.017736000	-0.583488000
C	-3.545615000	-1.581954000	0.939566000
C	4.643522000	1.362524000	0.957683000
C	5.112778000	-2.209835000	0.340764000
C	-3.464631000	-3.116125000	2.779801000
H	-3.117821000	-3.412481000	3.769992000
C	3.594433000	-4.135512000	-1.080809000
H	3.039859000	-4.905830000	-1.616986000
C	-3.980132000	-0.492819000	-0.925190000
C	3.879259000	-1.885616000	-0.302928000
C	4.567419000	0.002717000	0.594289000
C	-2.293275000	2.739189000	-2.864076000
H	-3.105023000	3.156403000	-3.480389000
C	6.692057000	-0.523866000	1.657931000
H	7.483631000	-1.218448000	1.939676000
C	3.119314000	-2.815106000	-1.037850000
C	-3.065570000	-1.889293000	2.225537000
C	-4.034637000	0.522120000	-1.898052000
C	-4.318102000	-3.987977000	2.062506000
C	-4.723150000	-1.710697000	-1.019613000
C	-4.438402000	-2.427670000	0.212427000
C	-5.527127000	-0.946668000	-3.172937000
C	1.639587000	-0.736977000	-4.442394000
H	0.589465000	-0.982739000	-4.645161000
H	2.142149000	-0.587722000	-5.409833000
H	1.656476000	0.220364000	-3.902061000
C	2.526024000	3.398508000	1.716028000
H	1.627632000	3.850978000	1.267379000
C	5.562204000	-3.541871000	0.274676000
H	6.490674000	-3.845634000	0.758463000
C	3.959297000	3.511587000	-0.909404000
H	4.758149000	4.060390000	-0.386804000
C	-5.497303000	-1.930024000	-2.174061000
H	-6.070815000	-2.848975000	-2.297984000
C	5.574281000	-0.959377000	0.924292000
C	0.294816000	-3.240866000	-1.887606000
H	0.682418000	-4.146043000	-2.381551000
C	4.796395000	-4.488147000	-0.421789000
C	-4.813117000	-3.653587000	0.793942000
H	-5.481347000	-4.339836000	0.273047000
C	2.073139000	2.509798000	2.890775000
H	1.339322000	1.767226000	2.555622000
H	1.608835000	3.133880000	3.668810000
H	2.930267000	1.986564000	3.337602000
C	-4.278954000	1.126026000	3.251042000
H	-3.843589000	1.822260000	2.518342000
H	-4.920797000	1.710928000	3.927339000
H	-4.914188000	0.412324000	2.709363000
C	-4.818666000	0.270704000	-3.036530000
H	-4.887161000	1.012512000	-3.832650000
C	-4.487728000	3.155793000	-0.806782000
H	-5.028942000	2.524144000	-0.083045000
C	2.909368000	4.510436000	-1.432944000
H	2.071427000	3.984205000	-1.912037000
H	3.364288000	5.174167000	-2.183216000
H	2.497556000	5.140670000	-0.633787000
C	5.788105000	1.765002000	1.668129000
H	5.925113000	2.807166000	1.951921000
C	-0.770529000	-1.325600000	3.991995000

H	-1.346614000	-1.985058000	4.660877000
C	-1.562773000	1.650794000	-3.677338000
H	-0.786335000	1.174458000	-3.065418000
H	-1.084480000	2.108739000	-4.557238000
H	-2.250337000	0.870634000	-4.025993000
C	2.353138000	-1.849399000	-3.647674000
H	3.391862000	-1.525164000	-3.474578000
C	-0.919612000	-2.713698000	-2.678795000
H	-1.276797000	-1.761811000	-2.266166000
H	-1.744611000	-3.437238000	-2.611068000
H	-0.690966000	-2.566764000	-3.742328000
C	2.391622000	-3.178494000	-4.423251000
H	2.946280000	-3.949067000	-3.872728000
H	2.893984000	-3.031612000	-5.391236000
H	1.380401000	-3.555520000	-4.629703000
C	6.788385000	0.828419000	2.017251000
C	3.463000000	4.524023000	2.195973000
H	4.342178000	4.114349000	2.709607000
H	2.926403000	5.157905000	2.917672000
H	3.808581000	5.170985000	1.379167000
C	0.208792000	-2.193765000	3.177960000
H	-0.320995000	-2.975690000	2.619851000
H	0.921988000	-2.683826000	3.858026000
H	0.773750000	-1.583762000	2.462805000
C	-1.314596000	3.869325000	-2.481028000
H	-1.815795000	4.703496000	-1.975119000
H	-0.834655000	4.266778000	-3.388961000
H	-0.535937000	3.482553000	-1.811218000
C	-3.181936000	0.399177000	4.056110000
H	-2.534247000	1.166357000	4.509244000
C	-0.019529000	-0.293920000	4.855888000
H	0.522607000	0.424437000	4.229502000
H	0.714343000	-0.811607000	5.491427000
H	-0.695003000	0.266406000	5.516139000
C	-5.467257000	3.538078000	-1.931446000
H	-4.982465000	4.171082000	-2.688633000
H	-6.305959000	4.114932000	-1.512551000
H	-5.883341000	2.653353000	-2.427994000
C	4.591823000	2.715795000	-2.068512000
H	5.336522000	1.995153000	-1.707740000
H	5.086887000	3.401659000	-2.771854000
H	3.822803000	2.162590000	-2.629613000
C	-0.101172000	-3.590579000	-0.439352000
H	0.748933000	-3.990542000	0.128066000
H	-0.899759000	-4.346662000	-0.448448000
H	-0.478983000	-2.703249000	0.082735000
C	-3.791039000	-0.473260000	5.167108000
H	-4.410486000	-1.273624000	4.740149000
H	-4.432487000	0.140555000	5.818017000
H	-3.021561000	-0.934439000	5.801029000
C	-3.989923000	4.408784000	-0.057395000
H	-3.236876000	4.154854000	0.699910000
H	-4.837735000	4.903363000	0.440237000
H	-3.544854000	5.138074000	-0.748247000
H	-1.597688000	2.644711000	1.130194000
H	-6.119710000	-1.115124000	-4.071839000
H	-4.604003000	-4.937532000	2.514316000
H	5.136466000	-5.522265000	-0.464987000
H	7.658265000	1.171840000	2.576135000
H	-1.287670000	2.085769000	1.945561000

2m^{L3}(closed-shell singlet)

Ti	1.428694000	0.163923000	0.233836000
Ti	-1.113079000	-0.436363000	-0.417854000
P	1.117292000	2.768541000	0.254822000
P	-2.144714000	-1.557744000	1.699546000
P	-2.582324000	1.615420000	-0.257955000
P	2.444828000	-2.169724000	-0.508815000
N	-2.264780000	-1.474264000	-1.595987000
N	2.610874000	0.291479000	1.786911000
N	0.264624000	0.223962000	-1.481905000
N	1.504225000	0.508478000	-1.642694000
H	0.195150000	-1.367469000	0.497294000
H	-0.290210000	0.444098000	1.072384000
H	-3.021568000	2.263715000	-1.441561000
H	-3.864422000	1.599940000	0.360403000
H	-2.116708000	2.775899000	0.404906000
H	-3.079258000	-2.054205000	-1.376260000
H	-2.149094000	-1.464687000	-2.613967000
H	-1.296883000	-1.559979000	2.825934000
H	-3.323451000	-1.162053000	2.399159000
H	-2.466266000	-2.944080000	1.729550000
H	2.291009000	3.559573000	0.168468000
H	0.433145000	3.358599000	-0.833306000
H	0.509684000	3.525563000	1.292179000
H	3.602711000	0.550407000	1.811497000
H	2.303826000	0.150288000	2.754264000
H	2.419240000	-3.317647000	0.320684000
H	1.800329000	-2.732215000	-1.631751000
H	3.778410000	-2.327015000	-0.969730000

2m'^{L3}(closed-shell singlet)

Ti	-1.119465000	-0.592681000	-0.071990000
Ti	1.256031000	0.681164000	-0.217593000
P	-3.235386000	1.046696000	-0.464663000
P	2.919139000	-1.261907000	-0.690477000
P	0.240721000	2.976451000	0.360936000
P	-0.164677000	-2.846219000	0.808051000
N	2.972851000	1.694180000	-0.197737000
N	-2.306119000	-1.677513000	-1.231326000
N	0.253120000	0.171602000	1.254155000
N	-0.878918000	-0.155997000	1.768987000
H	0.453529000	-0.734662000	-1.143464000
H	-0.413150000	0.976671000	-1.025271000
H	0.874028000	3.898074000	1.239935000
H	-0.215245000	3.958109000	-0.559333000
H	-0.969307000	2.852741000	1.080868000
H	3.921765000	1.309567000	-0.190466000
H	3.068452000	2.678585000	0.066659000
H	3.235172000	-1.550144000	-2.044708000
H	4.265299000	-1.234081000	-0.237129000
H	2.661749000	-2.605630000	-0.327596000
H	-4.496392000	0.444455000	-0.233502000
H	-3.578930000	2.324082000	0.059138000
H	-3.440684000	1.358259000	-1.825973000
H	-3.179648000	-2.159637000	-0.995159000
H	-2.006949000	-2.017197000	-2.151025000
H	0.485856000	-3.836048000	0.019995000
H	0.753837000	-2.829064000	1.883458000
H	-1.107329000	-3.731934000	1.388144000

TS$_{IJ}$^{L3}(closed-shell singlet)

Ti	-1.643668000	-0.361538000	0.078148000
Ti	1.988392000	-0.362973000	0.612634000
N	0.216546000	-0.977128000	0.478972000
N	0.265771000	0.301918000	-0.010400000
N	3.181431000	-0.518502000	2.140207000
N	-2.402667000	-1.797655000	-0.997030000
P	2.814802000	-1.408329000	-1.522173000
P	2.702829000	2.025686000	0.087149000
P	-2.093991000	1.791514000	-1.134040000
P	-4.146921000	-0.263670000	0.919266000
H	-1.897887000	0.809080000	1.416812000
H	-1.749712000	-0.192899000	1.830795000
H	1.767428000	-1.425639000	-2.468445000
H	3.835593000	-0.920647000	-2.386011000
H	3.199830000	-2.773974000	-1.648709000
H	3.131776000	-1.321598000	2.778975000

H	3.792373000	0.177101000	2.574994000
H	2.900250000	3.009170000	1.102165000
H	3.852593000	2.418505000	-0.656145000
H	1.761555000	2.754728000	-0.668548000
H	-3.352469000	2.445748000	-1.095452000
H	-1.313688000	2.896728000	-0.731164000
H	-1.906989000	1.983204000	-2.539276000
H	-3.339773000	-2.164612000	-1.168664000
H	-1.755391000	-2.300283000	-1.617356000
H	-5.137343000	0.589385000	0.347772000
H	-4.992265000	-1.408649000	0.936422000
H	-4.358155000	0.125454000	2.259374000

TS'_{IJ}^{L3} (closed-shell singlet)

Ti	1.761340000	-0.576117000	-0.401680000
Ti	-1.846613000	0.157320000	-0.200031000
P	2.856257000	1.720441000	-0.341860000
P	-1.877376000	2.707662000	0.076926000
P	-2.764756000	-2.216904000	-0.519053000
P	2.167051000	-1.135503000	2.017431000
N	-3.118153000	0.209678000	1.300963000
N	3.029973000	-1.285379000	-1.694257000
N	0.138086000	0.474162000	-0.166032000
N	-0.101814000	-0.859573000	-0.324006000
H	-2.288650000	-0.157876000	-1.883054000
H	-2.102261000	0.979604000	-1.744509000
H	3.356616000	2.373397000	-1.507739000
H	1.997217000	2.757622000	0.075923000
H	3.969789000	2.090702000	0.465211000
H	2.922309000	-2.221261000	-2.104091000
H	3.768271000	-0.809329000	-2.218184000
H	3.146448000	-0.580071000	2.888014000
H	1.024267000	-0.767104000	2.758206000
H	2.301634000	-2.460734000	2.521504000
H	-0.846180000	3.386253000	-0.607851000
H	-2.956701000	3.434665000	-0.482034000
H	-1.809825000	3.500475000	1.272273000
H	-3.322052000	1.017291000	1.896101000
H	-3.636200000	-0.584970000	1.685975000
H	-1.969743000	-3.038205000	-1.346215000
H	-3.049317000	-3.219559000	0.467848000
H	-3.983911000	-2.395025000	-1.218082000