

ELECTRONIC SUPPORTING INFORMATION

Can the pentamethylcyclopentadienyl ligand act as a proton-relay in *f*-element chemistry?
Insights from a joint experimental/theoretical study.

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I. Determination of rate constants.

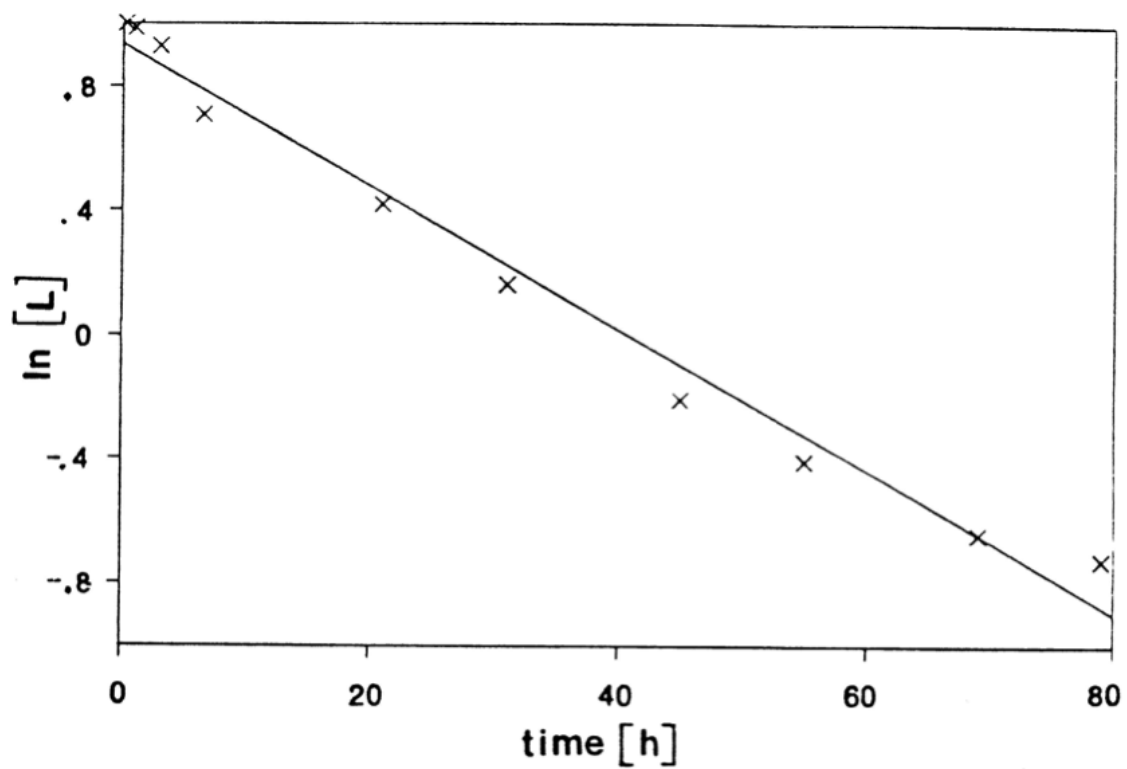


Figure S1. Plot of $\ln[\text{methylallene}]$ vs. t in cyclohexane- d_{12}

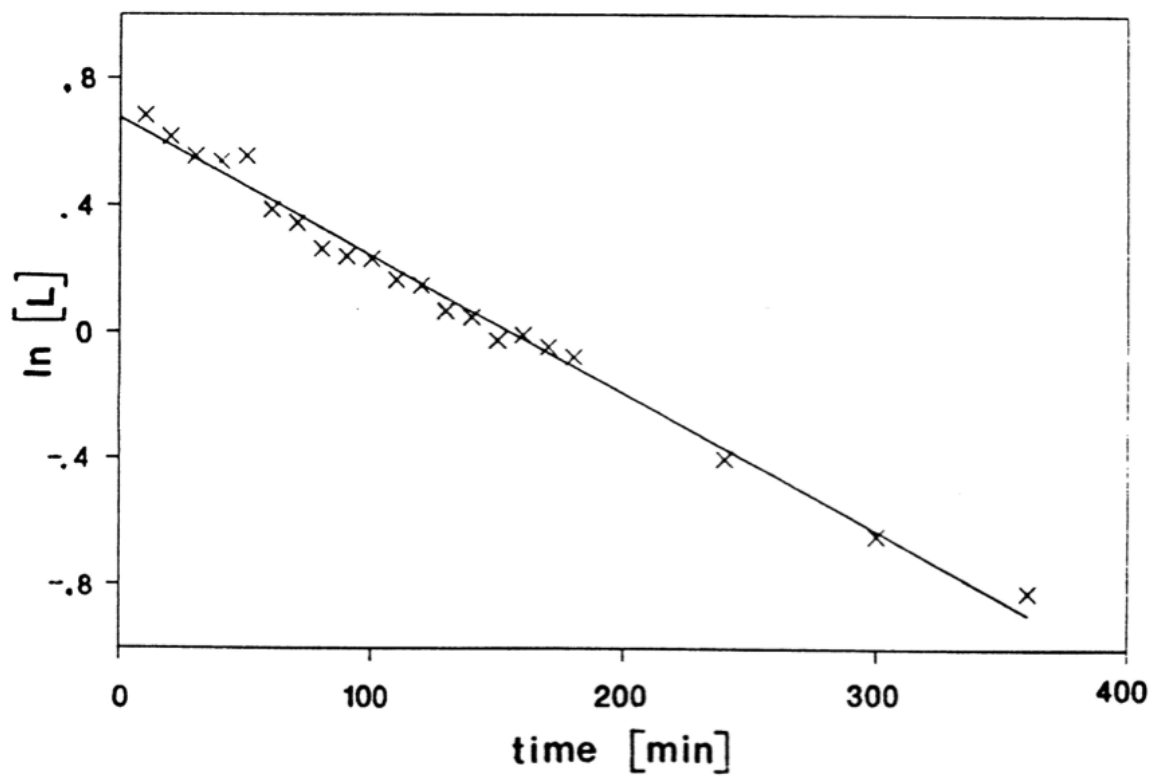


Figure S2. Plot of $\ln[\text{methylallene}]$ vs. t in benzene- d_6

II. Crystallographic data.

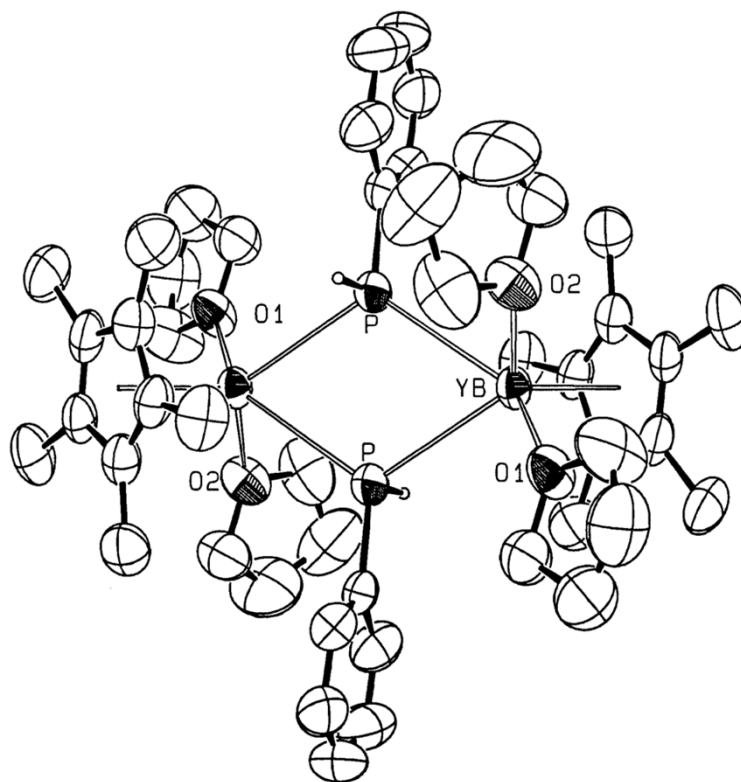


Figure S3. ORTEP diagram of $[\text{Yb}(\text{C}_5\text{Me}_5)(\mu\text{-PHC}_6\text{H}_5)(\text{THF})_2]_2$. The heavy atoms are refined anisotropically, 50% ellipsoids, and the hydrogen atom on phosphorus was located and refined isotropically, arbitrary ellipsoid. All other hydrogens are placed in calculated positions but not refined.

Table S1. Selected distances (Å) and angles ($^\circ$) for $[\text{Yb}(\text{C}_5\text{Me}_5)(\mu\text{-PHC}_6\text{H}_5)(\text{THF})_2]_2$.

Yb-Cp^(a)	2.43	Yb-P	2.967(2)
<Yb-C(Cp)>	2.71(3)	Yb-P'^(b)	3.066(2)
<Yb-C(Cp)>	2.71(3)	Yb-O(1)	2.445(7)
<Yb-C(Cp)>	2.71(3)	Yb-O(2)	2.497(7)
<Yb-C(Cp)>	2.71(3)	P-C(aryl)	1.834(9)
<C(Cp)-C(Cp)>	1.41(3)	P...P^(c)	3.301
<C(Cp)-C(Me)>	1.53(1)	Cp-Yb-P	112.5
<C(Cp)-C(Cp)>	1.41(3)	Cp-Yb-P'	121.8
<C(Cp)-C(Me)>	1.53(1)	Cp-Yb-O(1)	109.9
Yb-P	2.967(2)	Cp-Yb-O(2)	118.4
Yb-P'^(b)	3.066(2)	P-Yb-P'	66.5(1)
Yb-O(1)	2.445(7)	P-Yb-O(1)	91.2(2)
Yb-O(2)	2.497(7)	P-Yb-O(2)	118.9(2)
P-C(aryl)	1.834(9)	O(1)-Yb-O(2)	77.4(3)
<C(Cp)-C(Cp)>	1.41(3)	Yb-P-C(aryl)	124.7(3)
<C(Cp)-C(Me)>	1.53(1)	Yb-P-Yb'	113.5(1)

(a) Cp denotes the centroid of C(1)-C(5)

(b) ' denotes atom at -x, -y, -z.

(c) Non-bonding distance.

III. Computed Electron Affinities.

Experimental and computed electron affinities of ethylene,[1] butadiene,[1] allene[2], propyne[2] and deprotonated allene[3,4] and propyne[3] have been reported, values shown in Table 1. In order to compare homogeneous values, we have computed the electron affinities of ethylene, allene, methylallene, propyne, but-2-yne, butadiene, and deprotonated allene and propyne at high level *ab initio* using the CBS-QB3 and W1U methodologies. Computed values for ethylene, butadiene, allenyl and propynyl anions match the experimental values with deviations of less 0.1 eV, especially at the W1U level. In contrary, large variations are observed for allene, dimethylacetylene and propyne. For allene and propyne, low precision for these experimental values are expected by the authors due to the equilibrium between allene and propyne in the measurement conditions.[3,4] For dimethylacetylene, experimental values correspond to vertical (diabatic) excitation.[5] The following trend of AEs for substrate of interest in the current study is ethylene (-1.555 eV); but-2-yne (-1.319 eV); buta-1,2-diene (-0.971 eV) ; *s-trans*-butadiene (-0.605 eV).

Table S2. Reported (experimental and calculated) and adiabatic calculated electron affinities in eV.

molecule	reported AE	AE calc. ^k	
		CBS-QB3 ⁱ	W1U ^j
C₂H₄	-1.55±0.1 ^a	-1.699	-1.555
	-1.78 ^b		
	-1.87 ^c		
	-1.8 ^d		
H₂C=C=CH₂	-1.9±0.1 ^e	-1.332	-1.317
H₂C=C=CHMe	n.a.	-0.978	-0.971
MeCCH	-2.8±0.1 ^e	-1.648	-1.642
MeCCMe	-3.43 ^f 3.6 ^{f2}	-1.321	-1.319
<i>trans</i>-C₄H₆	-0.62±0.05 ^a	-0.692	-0.695
H₂CCCH⁻	0.893±0.025 ^g	0.889	0.895
	0.918±0.008 ^h		
MeCC⁻	2.718±0.008 ^g	2.823	2.799

^a ref. [1]; ^b ref. [6]; ^c ref. [7]; ^d ref. [8]; ^e ref. [2]; ^f ref. [5]; ^{f2} ref. [9]; ^g ref. [3]; ^h ref. [4]; ⁱ ref. [10]; ^j ref. [11]; ^k Electron affinities have computed using the electron convention: $\Delta_f H^\circ(e^-, 0\text{ K}) = 0\text{ kcal mol}^{-1}$, energies have been corrected by zero-point vibrational energy (ZPE).

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 [10] (a) J. A. Montgomery Jr., M. J. Frisch, J. W. Ochterski and G. A. Petersson, *J. Chem. Phys.*, 1999, **110**, 2822-2827. (b) J. A. Montgomery Jr., M. J. Frisch, J. W. Ochterski and G. A. Petersson, *J. Chem. Phys.*, 2000, **112**, 6532-6542.
 [11] (a) J. M. L. Martin and G. de Oliveira, *J. Chem. Phys.*, 1999, **111**, 1843-1856. (b) S. Parthiban and J. M. L. Martin, *J. Chem. Phys.* **2001**, 114, 6014-6029.

IV. Selectivity of C-H bond activation.

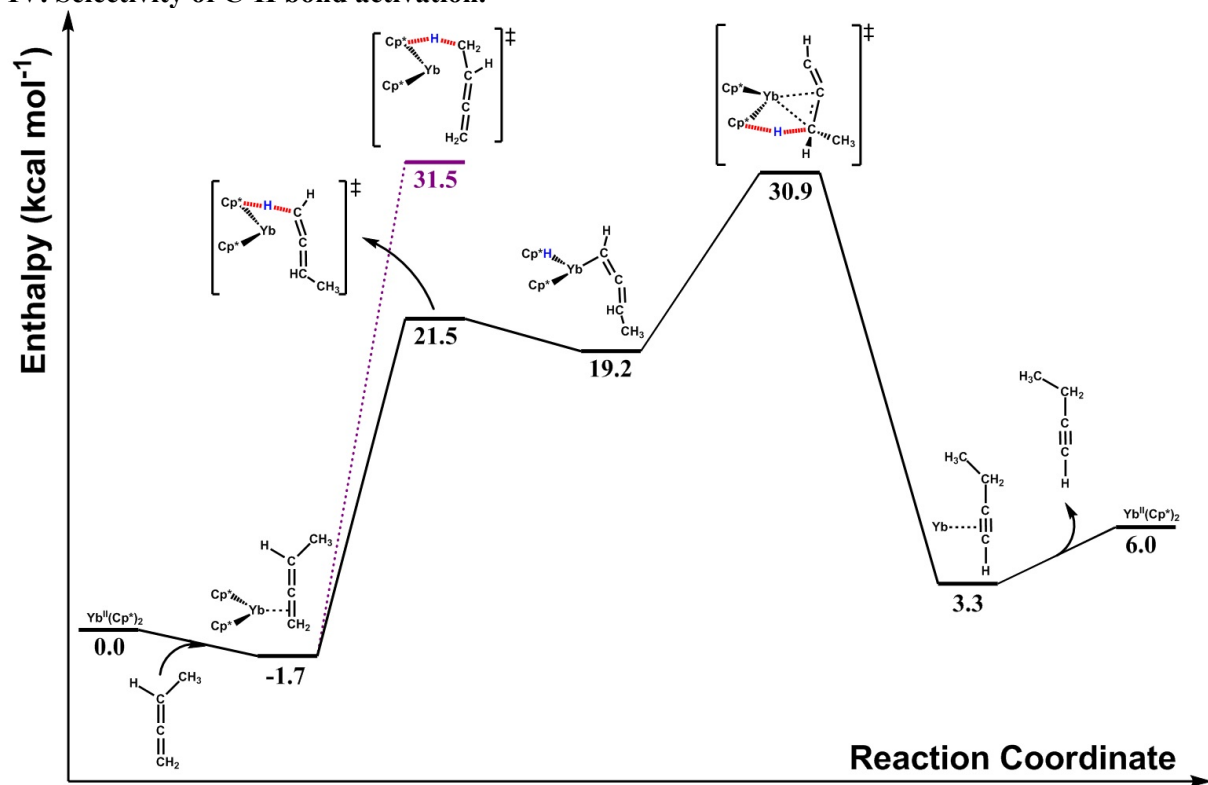


Figure S4. Energy profile for alternative C-H activation of buta-1,2-diene by $(\text{Me}_5\text{C}_5)_2\text{Yb}$.

V. Energies (au) and Cartesian coordinates of optimized complexes and organic molecules.

V.A Electron Affinities

C_2H_4

CBS-QB3 Energy -78.413594
C 0.00000000 0.00000000 0.06145654
C 0.00000000 0.00000000 1.38854346
H 0.92208058 0.00000000 -0.51060403
H -0.92208058 0.00000000 -0.51060403
H 0.92208058 0.00000000 1.96060403
H -0.92208058 0.00000000 1.96060403
WIU Energy -78.551637
C 0.00000000 0.00000000 0.06304716
C 0.00000000 0.00000000 1.38695284
H 0.92023731 0.00000000 -0.50729260
H -0.92023731 0.00000000 -0.50729260
H 0.92023731 0.00000000 1.95729260
H -0.92023731 0.00000000 1.95729260

$[C_2H_4]^-$

CBS-QB3 Energy -78.351148
C 0.00000000 0.00000000 0.00424663
C 0.00000000 0.00000000 1.44575337
H 0.92476860 0.00000000 -0.57130662
H -0.92476860 0.00000000 -0.57130662
H 0.92476860 0.00000000 2.02130662
H -0.92476860 0.00000000 2.02130662
WIU Energy -78.494464
C 0.00000000 0.00000000 0.00703147
C 0.00000000 0.00000000 1.44296853
H 0.92213290 0.00000000 -0.56655187
H -0.92213290 0.00000000 -0.56655187
H 0.92213290 0.00000000 2.01655187
H -0.92213290 0.00000000 2.01655187

$H_2C=C=CH_2$

CBS-QB3 Energy -116.416502
C -1.99534877 0.74007398 -0.00043498
C -3.29779962 0.74073706 0.00033555
H -3.86278182 -0.18567123 -0.03079767
H -3.86179515 1.66772356 0.03212859
C -0.69289803 0.73927880 -0.00121054
H -0.12787651 0.70748415 0.92515106
H -0.12894210 0.77040369 -0.92824400
WIU Energy -116.622875
C -1.99534879 0.74006923 -0.00042730
C -3.29529983 0.74073467 0.00034841
H -3.85886034 -0.18385397 -0.03073962
H -3.85786976 1.66590521 0.03204718
C -0.69539786 0.73927051 -0.00120849
H -0.13179588 0.70754617 0.92333306
H -0.13286953 0.77035818 -0.92642525

$[H_2C=C=CH_2]^-$

CBS-QB3 Energy -116.367538
C -1.99534867 0.74019585 -0.00018192
C -3.33725870 0.74072826 0.00047511
H -3.94990491 -0.07694596 -0.41820250
H -3.94883530 1.55908798 0.41935902
C -0.65343921 0.73920338 -0.00117079
H -0.04044735 1.10121763 0.84286002
H -0.04220785 0.37654286 -0.84621094
WIU Energy -116.574468
C -1.99534857 0.74019050 -0.00018406
C -3.33573589 0.74072784 0.00047161
H -3.94383157 -0.07603471 -0.41650598
H -3.94275870 1.55817238 0.41765872
C -0.65496196 0.73919540 -0.00116701
H -0.04652598 1.09959416 0.84183631
H -0.04827933 0.37818444 -0.84518159

$H_2C=C=CHMe$

CBS-QB3 Energy -155.641678
C -3.26518720 0.72306654 -0.00041820
C -1.96094780 0.75143103 -0.00001098
C -0.65749957 0.77659789 0.00014451
C -4.10797766 -0.53775463 -0.04425963
H -3.79116642 1.67520853 0.03228087
H -0.08937647 0.75677898 0.92584031
H -0.09035060 0.82066663 -0.92530865
H -5.17051175 -0.28939587 -0.03542981
H -3.90791121 -1.12063612 -0.94725010
H -3.90759734 -1.18210197 0.81587168
WIU Energy -155.917089
C -3.26358999 0.72110546 -0.00049672
C -1.96197793 0.74990216 -0.00006639
C -0.66099063 0.77603284 0.00012655
C -4.10572831 -0.53638783 -0.04421363
H -3.78799534 1.67148091 0.03215402
H -0.09436718 0.75666945 0.92400711
H -0.09533681 0.82045343 -0.92348013
H -5.16554552 -0.28738747 -0.03536039
H -3.90665543 -1.11835188 -0.94498762
H -3.90633885 -1.17965607 0.81377720

$[H_2C=C=CHMe]^-$

CBS-QB3 Energy -155.605732
C -3.11910809 0.49831403 0.13311892
C -1.88070057 0.40253557 -0.41102223
C -0.63168744 0.88954498 -0.16090505
C -4.21135582 -0.52804456 -0.05164677
H -3.41187775 1.37957266 0.73428591
H -0.29141817 1.17294992 0.84962511
H 0.12171296 1.00471820 -0.94286290
H -5.15916253 -0.09846122 -0.43538942
H -3.87726718 -1.28525581 -0.77126378
H -4.48766140 -1.06201278 0.87752021
WIU Energy -155.881132
C -3.11954955 0.49782196 0.12835583
C -1.88152616 0.40468576 -0.40661995
C -0.63551819 0.89342754 -0.15877914
C -4.20765874 -0.52925369 -0.05180598
H -3.41417901 1.38043617 0.72062890
H -0.29625693 1.16616690 0.85082294
H 0.11536233 1.00604437 -0.93858527
H -5.15401500 -0.09952821 -0.42858565
H -3.87980945 -1.28574604 -0.77129538
H -4.47537530 -1.06019375 0.87732370

MeCCH

CBS-QB3 Energy -116.417702
C -2.00827782 0.74360222 0.00018669
C -3.20916752 0.74668850 0.00025171
H -4.27122233 0.74939754 0.00030447
C -0.55115365 0.73971828 0.00001608
H -0.15791577 1.27971439 -0.86587647
H -0.15787126 1.21800210 0.90144111
H -0.16207164 -0.28171603 -0.03567259
WIU Energy -116.624496
C -2.00719604 0.74348731 0.00020937
C -3.20611449 0.74666069 0.00024861
H -4.26686443 0.74950165 0.00028819
C -0.55237174 0.73970067 0.00002014
H -0.16042935 1.27861664 -0.86411194
H -0.16034278 1.21702720 0.89959681
H -0.16436116 -0.27958716 -0.03560019

$[MeCCH]^-$

CBS-QB3 Energy -116.357139
C -2.03065945 1.44509682 0.02482872
C -3.25682855 1.08364722 0.01250362
H -3.67136280 0.04154827 -0.02488692

C	-0.67990310	0.79226765	0.00184379
H	-0.07612144	1.11105455	-0.86394207
H	-0.07592093	1.04978546	0.88764776
H	-0.72688372	-0.32799297	-0.03734391

WIU Energy -116.564164

C	-2.02434254	1.43691739	0.02890316
C	-3.24959696	1.08422531	0.01509779
H	-3.68616673	0.05932011	-0.02535716
C	-0.67624820	0.78809399	0.00126124
H	-0.07838109	1.11274265	-0.86163165
H	-0.07683370	1.04119687	0.88675557
H	-0.72611078	-0.32708932	-0.04437794

MeCCMe

CBS-QB3 Energy -155.648913

C	-1.26134645	0.18137272	-0.00027195
C	-0.05838392	0.18175398	-0.00002408
C	-2.72012051	0.18059484	-0.00016152
H	-3.11637269	1.01565206	0.58538176
H	-3.11619669	0.26979682	-1.01621286
H	-3.11546498	-0.74429937	0.43050459
C	1.40038997	0.18218130	0.00014729
H	1.79644769	-0.69040595	0.52827532
H	1.79646629	0.16133504	-1.01960016
H	1.79593028	1.07597155	0.49196160

WIU Energy -155.924336

C	-1.26035184	0.18165978	-0.00012335
C	-0.05938182	0.18188236	0.00053501
C	-2.71690261	0.18059108	-0.00021472
H	-3.11219503	1.01383373	0.58404379
H	-3.11168954	0.26954064	-1.01419203
H	-3.11102052	-0.74241873	0.42949840
C	1.39716320	0.18215289	0.00016283
H	1.79219598	-0.68863154	0.52705011
H	1.79172264	0.16131718	-1.01758298
H	1.79180854	1.07402562	0.49082294

[MeCCMe]

CBS-QB3 Energy -155.600367

C	-1.16957423	0.39000746	-0.33843504
C	-0.15011915	-0.02654293	0.33895002
C	-2.63887497	0.21914346	-0.06203579
H	-3.15240707	1.18992037	0.03222521
H	-3.15167275	-0.30255731	-0.88652138
H	-2.85045809	-0.35382936	0.86861302
C	1.31903450	0.14360492	0.06202847
H	1.83195553	-0.82738255	-0.03329245
H	1.53077923	0.71727997	-0.86821397
H	1.83268600	0.66430898	0.88668191

WIU Energy -155.875794

C	-1.17365575	0.38575229	-0.32844164
C	-0.14591694	-0.02256346	0.32956305
C	-2.63764758	0.21876246	-0.05853186
H	-3.14663560	1.18781581	0.03588983
H	-3.14632176	-0.29958116	-0.88295135
H	-2.85186694	-0.35368800	0.86813253
C	1.31796057	0.14404265	0.05844422
H	1.82645379	-0.82518408	-0.03680707
H	1.53152005	0.71687492	-0.86808135
H	1.82745915	0.66172157	0.88278364

trans-C₄H₆

CBS-QB3 Energy -155.662271

C	0.00687321	0.00000000	0.07126555
C	0.02233414	0.00000000	1.40834470
C	1.23340286	0.00000000	2.21665530
C	1.24886379	0.00000000	3.55373445
H	0.92641688	0.00000000	-0.50552156
H	-0.92138479	0.00000000	-0.48732123
H	-0.92025456	0.00000000	1.95205498
H	2.17599156	0.00000000	1.67294502
H	0.32932012	0.00000000	4.13052156
H	2.17712179	0.00000000	4.11232123

WIU Energy -155.938084

C	0.00856421	0.00000000	0.07582123
C	0.02365037	0.00000000	1.40956173
C	1.23208663	0.00000000	2.21543827
C	1.24717279	0.00000000	3.54917877
H	0.92638897	0.00000000	-0.49915496
H	-0.91782599	0.00000000	-0.48110135
H	-0.91688593	0.00000000	1.95194370
H	2.17262293	0.00000000	1.67305630
H	0.32934803	0.00000000	4.12415496
H	2.17356299	0.00000000	4.10610135

[trans-C₄H₆]

CBS-QB3 Energy -155.636837

C	-0.00133594	0.00000000	-0.00448597
C	0.06137027	0.00000000	1.39633323
C	1.19436673	0.00000000	2.22866677
C	1.25707294	0.00000000	3.62948597
H	0.89934371	0.00000000	-0.61552770
H	-0.95182088	0.00000000	-0.52921429
H	-0.90151113	0.00000000	1.92054872
H	2.15724813	0.00000000	1.70445128
H	0.35639329	0.00000000	4.24052770
H	2.20755788	0.00000000	4.15421429

WIU Energy -155.912555

C	0.00045798	0.00000000	0.00007113
C	0.06213438	0.00000000	1.39799187
C	1.19360262	0.00000000	2.22700813
C	1.25527902	0.00000000	3.62492887
H	0.89879665	0.00000000	-0.60966287
H	-0.94771682	0.00000000	-0.52292175
H	-0.89851651	0.00000000	1.92014464
H	2.15425351	0.00000000	1.70485536
H	0.35694035	0.00000000	4.23466287
H	2.20345382	0.00000000	4.14792175

H₂CCCH

CBS-QB3 Energy -115.774568

C	-2.02621023	0.73316423	0.20173477
C	-3.37414046	0.74168684	-0.02661545
H	-3.92185583	-0.18439724	-0.15115967
H	-3.92080085	1.67470632	-0.08801620
C	-0.82134987	0.72555344	0.40563427
H	0.22585623	0.71891341	0.58359428

WIU Energy -115.979581

C	-2.02711383	0.73317011	0.20158701
C	-3.37219194	0.74167792	-0.02635592
H	-3.91876293	-0.18239879	-0.15063794
H	-3.91771123	1.67267333	-0.08763520
C	-0.82431371	0.72556842	0.40523571
H	0.22159263	0.71893601	0.58297833

[H₂CCCH]

CBS-QB3 Energy -115.807223

C	-1.96590516	0.73754058	0.07184421
C	-3.31493155	0.74071467	0.00096059
H	-3.89243952	-0.18189971	-0.05483657
H	-3.89138848	1.66564440	0.00790402
C	-0.69003175	0.73950275	-0.00704980
H	-0.08380454	0.70812430	0.90634955

WIU Energy -116.013752

C	-1.96818872	0.73754515	0.07054564
C	-3.31419164	0.74094795	-0.00615906
H	-3.88852885	-0.18034304	-0.05178577
H	-3.88742187	1.66390029	0.01099864
C	-0.69541472	0.73921173	-0.00175822
H	-0.08475520	0.70836492	0.90333077

MeCC

CBS-QB3 Energy -115.705438

C	-1.99698203	0.88703998	0.00564749
C	-3.21677488	0.61891090	-0.00431021
C	-0.54747438	0.76930268	0.00097006
H	-0.11259336	1.26074875	-0.87404442
H	-0.11225842	1.19772202	0.90837733

H -0.26037593 -0.28771532 -0.03629324
WIU Energy -115.911755
C -1.99365235 0.88761242 0.00638571
C -3.21340148 0.62408161 -0.00467394
C -0.54828186 0.76896407 0.00084967
H -0.11360247 1.25776649 -0.87295301
H -0.11289686 1.19452375 0.90691801
H -0.26462399 -0.28693933 -0.03617943

[MeCC]

CBS-QB3 Energy -115.809187
C -2.02984620 0.74422996 0.00017954

C -3.27210638 0.74636125 0.00026808
C -0.56298108 0.73983094 0.00001213
H -0.12565111 1.27670221 -0.86129977
H -0.12563393 1.21531068 0.89666855
H -0.13024030 -0.27642603 -0.03548153
WIU Energy -116.015116
C -2.02584130 0.74394039 0.00016594
C -3.26390302 0.74657304 0.00027777
C -0.56212991 0.73978730 0.00001008
H -0.13006971 1.27571086 -0.85961725
H -0.13005322 1.21443720 0.89492095
H -0.13446184 -0.27443980 -0.03541049

V.B Reactivity: Organic molecules

H₂C=C=CHMe

E: -155.919645079 ; H: -155.829368 ; G: -155.862278
C -3.25442316 0.69604592 -0.20762648
C -1.95856469 0.74317662 -0.02971873
C -0.66438707 0.78895248 0.14926710
C -4.10402870 -0.53514499 -0.04212064
H -3.76542393 1.61530355 -0.49868024
H -0.23245755 1.01999426 1.12099140
H 0.02970545 0.59929245 -0.66710201
H -4.87434881 -0.37745682 0.72220153
H -4.62363505 -0.77876420 -0.97647234
H -3.50096249 -1.39753726 0.25072041

C₂H₄

E: -78.5600140988 ; H: -78.504836 ; G: -78.529700
C 0.00000000 0.00000000 0.06006440
C 0.00000000 0.00000000 1.38993560
H 0.92412584 0.00000000 -0.51236355
H -0.92412584 0.00000000 -0.51236355
H 0.92412584 0.00000000 1.96236355
H -0.92412584 0.00000000 1.96236355

MeCCMe

E: -155.922666671 ; H: -155.831594 ; G: -155.867013
C -1.26497787 0.18121757 0.00046244
C -0.05475284 0.18169237 0.00054149
C -2.72180422 0.18058392 -0.00012815
H -3.12050349 1.04869819 0.53683476
H -3.11933013 0.21146561 -1.02087541
H -3.11969462 -0.71893731 0.48304749
C 1.40207345 0.18220553 0.00014126
H 1.80060477 -0.72006649 0.47762698
H 1.79970879 0.21990533 -1.02033485
H 1.80002415 1.04718928 0.54268401

H₂

E: -1.17751650801 ; H: -1.164060 ; G: -1.178853
H 0.313535023 -3.22349565 0.
H -0.429867423 -3.22349565 0.

OE_t₂

E: -233.586122212 ; H: -233.441193 ; G: -233.478394
O 0.0. 0. -0.2614700405
C -1.175654106 0. 0.5170084759
H -1.1992256001 -0.8862195469 1.1757320356
H -1.1992256001 0.8862195469 1.1757320356
C -2.3725496795 0. -0.4131638997
H -2.3598270149 0.8859761273 -1.0544198027
H -2.3598270149 -0.8859761273 -1.0544198027
H -3.3047602516 0. 0.1602158482
C 1.175654106 0. 0.5170084759
H 1.1992256001 0.8862195469 1.1757320356
H 1.1992256001 -0.8862195469 1.1757320356
C 2.3725496795 0. -0.4131638997
H 3.3047602516 0. 0.1602158482
H 2.3598270149 -0.8859761273 -1.0544198027

H 2.3598270149 0.8859761273 -1.0544198027

THF

E: -232.372952201 ; H: -232.249610 ; G: -232.284258
O 4.5361522244 0.3643078874 1.1675781652
C 4.2244670282 -0.7812834367 1.937818673
C 5.8667171067 0.7184317141 1.5106922925
H 4.6974617296 -1.6828843797 1.509692896
H 3.1398361003 -0.9194506792 1.9160306598
C 4.7918437417 -0.4799502424 3.3261639938
C 6.0641449755 0.3291292145 2.9959546404
H 5.9856094184 1.7886204016 1.3173115636
H 6.5822428983 0.1755388313 0.8719474441
H 4.9952854959 -1.382296452 3.9099670791
H 4.0823340831 0.1336008291 3.8898174827
H 6.1594161406 1.2071135667 3.6405493645
H 6.9701180573 -0.2703122549 3.1261787453

C₆H₅PH₂

E: -239.321912269 ; H: -239.206053 ; G: -239.245358
P 0.49485 -0.06017 0.089986
H 1.547366 -1.017817 -0.0833
H 1.010756 0.787402 -0.947681
C 1.232639 0.842971 1.539399
C 0.349435 1.436153 2.449014
C 2.611012 0.948528 1.769315
C 0.83103 2.132962 3.557826
H -0.722738 1.349075 2.29036
C 3.092175 1.637176 2.880017
H 3.311636 0.491292 1.075703
C 2.202863 2.233439 3.775247
H 0.132691 2.590271 4.253502
H 4.163587 1.709994 3.047113
H 2.580241 2.770793 4.640966

PhCCH

E: -308.274409610 ; H: -308.157204 ; G: -308.194352
C 0.0. -2.0201155987
C 0.0. -3.2312307519
H 0.0. -4.2976190231
C 0.0. -0.5926970307
C -1.2117621678 0. 0.1200093554
C 1.2117621678 0. 0.1200093554
C -1.2070645414 0. 1.5107015734
H -2.1484165019 0. -0.4289026805
C 1.2070645414 0. 1.5107015734
H 2.1484165019 0. -0.4289026805
C 0.0. 2.2100997468
H -2.1496852635 0. 2.0508785061
H 2.1496852635 0. 2.0508785061
H 0.0. 3.296457867

HCp*

E: -390.567826011 ; H: -390.321927 ; G: -390.372204

H 2.3327797968 -1.2658350235 0.2585763265
C 4.3065678824 -0.3717767185 -1.8777721138
C 5.0543249846 -0.2176215973 -0.6091813116
C 3.248111572 -1.1916713229 -1.6777121885
C 4.4488615378 -0.9445080956 0.3593297527
C 3.2460313018 -1.6408586728 -0.2344966645
C 2.2031736469 -1.6308324699 -2.6501829987
H 2.2039469004 -2.7206781345 -2.7867540329
H 1.1951667083 -1.3610735042 -2.3079630023
H 2.3454478208 -1.1796256006 -3.6358305625
C 3.2809310143 -3.1675705512 -0.0717484534
H 4.1752045121 -3.5809753462 -0.5491503374
H 3.2938722604 -3.4551678582 0.9845807647

H 2.4030137573 -3.6348663772 -0.5294683853
C 4.8249494348 -1.0922368425 1.7969742744
H 5.0675507576 -2.1328958783 2.0511562165
H 5.694602191 -0.4831219172 2.0576840895
H 4.0031991893 -0.7931642658 2.4611591055
C 6.2783141709 0.6366501857 -0.496692202
H 6.0662042688 1.6791328853 -0.7655885822
H 6.6894377289 0.6339163414 0.5158452229
H 7.0696629854 0.2931518962 -1.1748094212
C 4.7178419085 0.3160556634 -3.1418568992
H 4.0524757663 0.0762212006 -3.974891419
H 4.7193057734 1.4069242123 -3.0229330895
H 5.7350201292 0.0319457914 -3.4393241082

V.C Reactivity: (Me₅C₅)₂Yb, buta-1,2-diene to but-2-yne

Yb (large core)

(Me₅C₅)₂Yb (lc)

E: -812.992442434 ; H: -812.522447 ; G: -812.609907

Yb 3.6599937471 1.6752017685 -0.0880863019
C 4.1433133898 -0.5925378749 -1.5428841223
C 5.4312563253 -0.1179746301 -1.1563821554
C 3.468174356 -1.0413018075 -0.3699638574
C 5.5521178409 -0.2736218857 0.2559408069
C 4.3388373341 -0.8442296356 0.741801529
C 1.8936012734 3.4719904568 0.9816561958
C 3.182224104 3.9459653041 1.3662879658
C 1.7709620756 3.6259445063 -0.430692047
C 3.8562188394 4.3928023849 0.1915562843
C 2.9837499014 4.1954271146 -0.9190139753
C 0.5338955026 3.3542401393 -1.242585716
H -0.1240311123 4.2332088875 -1.2889435875
H 0.7664660406 3.086392917 -2.2797257415
H -0.0673681313 2.5389027317 -0.8241401933
C 3.24773397 4.627708922 -2.3356328801
H 4.3130257817 4.5899747823 -2.5909558614
H 2.7165210404 4.0066709484 -3.0661410826
H 2.9222899453 5.6622241762 -2.5128850263
C 5.1992033279 5.0695022259 0.1501175719
H 5.8685586481 4.714585574 0.9422838407
H 5.7155005084 4.9135240823 -0.8041870566
H 5.1118395582 6.1570238183 0.2816080908
C 3.6903662129 4.0735943458 2.7766026682
H 3.4155079045 5.0398082776 3.2219905692
H 3.2825526992 3.3004919296 3.4380097244
H 4.7829214412 4.0057332997 2.8340584149
C 0.8084279276 3.0098734277 1.9154422527
H 0.16985129 3.8425317378 2.2416958729
H 0.143268957 2.273290349 1.450030323
H 1.2115654378 2.5527806047 2.8263339473
C 2.1239406814 -1.7156631178 -0.3301240546
H 2.209090961 -2.8030917554 -0.4637936001
H 1.6078652787 -1.5605837203 0.6244276389
H 1.4553817601 -1.3579905129 -1.1217669301
C 4.0763200939 -1.2829770518 2.1567162223
H 4.4068046859 -2.3165846339 2.3298592955
H 4.6043142346 -0.6621287535 2.8897222442
H 3.0108236249 -1.2513100372 2.4119531757
C 6.7875374903 -0.0028672165 1.0705580756
H 7.4390972935 -0.8859086334 1.1280177604
H 7.3957227739 0.8043309868 0.6466761101
H 6.5529526002 0.2765509032 2.1042690858
C 6.5161771832 0.3446041402 -2.0902068821
H 6.1136397427 0.8167063511 -2.993805042
H 7.1906825878 1.0689080756 -1.6192383561
H 7.1447321331 -0.4904291442 -2.4295639389
C 3.6365220604 -0.7172190562 -2.9539562829

H 2.5438897007 -0.6511140076 -3.0120818242
H 4.0436842822 0.0583039408 -3.6129555838
H 3.9133323883 -1.681726635 -3.4018515665

A_Yb (lc)

E: -968.917785591 ; H: -968.354446 ; G: -968.460727

C 0.4292879582 -0.0979383856 2.1440002366
C 0.9926025215 0.3110777447 3.2520924011
Yb -2.5785302993 -1.5248889276 2.5017117622
C -3.3806121226 0.9398938769 3.4803947692
C -3.4443212671 1.0815401393 2.0637889054
C -4.3936252242 0.0196292705 3.877799472
C -4.4920609563 0.2434156568 1.5844028036
C -5.0835698005 -0.4079257126 2.7061451213
C -0.9888574636 -3.8178792822 2.5379404469
C -1.6851986062 -3.8006956138 3.7811575815
C -1.9432541511 -4.0356000063 1.5025646592
C -3.0672752988 -4.0261600156 3.5169387391
C -3.2277409766 -4.165762785 2.1073296955
C -4.1367339445 -4.237488889 4.551531581
H -3.9549131398 -3.6569936075 5.4627554213
H -5.1295095819 -3.9589759455 4.1827187934
H -4.1992607338 -5.2912248369 4.8579997054
C -4.4961561259 -4.5447212371 1.3943944366
H -4.5916720306 -5.6346715635 1.288098719
H -5.3877404561 -4.2010161219 1.9283269761
H -4.5461582004 -4.1288167932 0.3811812692
C -1.6461340968 -4.2461857424 0.0430245519
H -2.4438750993 -3.8629237186 -0.6045669137
H -0.7149340114 -3.7593662341 -0.2696441339
H -1.5342699128 -5.3116344078 -0.2022788494
C 0.506918562 -3.803808918 2.3841287784
H 0.9951603128 -3.0443426073 3.0064236149
H 0.9472300283 -4.7700536952 2.6673085444
H 0.8140277586 -3.6205256233 1.3486513652
C -1.0453800725 -3.7151078794 5.1396780856
H -0.739083169 -4.703490383 5.511160168
H -0.1415634364 -3.0940362833 5.1346317561
H -1.7237836991 -3.2975042323 5.892274039
C -6.3255320921 -1.2534742031 2.6752028305
H -6.4097218728 -1.8388933435 1.7532419616
H -6.3670673907 -1.9581358166 3.5123057323
H -7.2332159931 -0.6366440368 2.7393246013
C -4.763860048 -0.3250574805 5.2937211675
H -5.5328864704 0.3527271172 5.6905184728
H -5.1635480405 -1.3408170636 5.3814785722
H -3.9072278229 -0.2553057769 5.9739490591
C -2.512038318 1.7451611343 4.4072413816
H -3.017225062 2.660987801 4.7454730153
H -2.241139357 1.1921333801 5.3151729307

H -1.5802116892 2.0635552136 3.926641256
C -2.6640852954 2.0693778773 1.2424810875
H -1.6542097052 2.2356481917 1.6349015613
H -2.5627180621 1.7506078023 0.1981278981
H -3.1550292985 3.0525004157 1.2158471463
C -4.9860943145 0.1687896746 0.1654508966
H -4.1846712667 0.3273646988 -0.5660069353
H -5.4436521763 -0.8006692378 -0.0619452899
H -5.750434853 0.9308295035 -0.0427420251
C 2.4156529145 0.7892584521 3.3595896423
H 2.4450047786 1.8181447665 3.7348556104
H 2.9750674659 0.1680724845 4.0677209483
H 2.923218534 0.7566795606 2.3935306766
C -0.1122508002 -0.4997621898 1.0159416309
H -0.0274305637 -1.5364902523 0.6921219137
H -0.597597199 0.2068994005 0.3449014396
H 0.3981347335 0.3146186866 4.1663163156

TS_A_Yb (lc)

E: -968.876579830 ; H: -968.318487 ; G: -968.420372
Yb 0.3600409071 0.3899111083 0.2745405354
H -2.6924264664 -2.4244183769 -0.3923225792
C -3.1451629633 -1.7013524857 0.295520146
C -2.1851148128 -0.5912605197 0.6089372589
C -2.3333508479 0.6889633079 0.524958184
C -2.1770779363 2.017290539 0.515216103
H -4.0776263077 -1.3438037813 -0.1548587488
H -3.4007682402 -2.2580588988 1.2042676154
H -1.0482356203 -0.9566185212 1.5944442217
H -2.4631124058 2.6257169 1.3703453501
H -1.9349008551 2.5450643995 -0.4048948368
C 0.0880743103 0.1258711515 3.1938076064
C -0.2071971755 -1.1972212094 2.6172008958
C 1.0870471492 -1.7015808086 2.1236924626
C 2.0537889776 -0.728422222 2.3321349789
C 1.4272117657 0.4166908328 2.9817250032
C 0.8533973112 -0.1816515392 -2.3610917508
C 2.145263255 -0.0338788046 -1.7780549201
C 2.3126125352 1.3374564516 -1.4256214642
C 1.1259634588 2.0359891694 -1.7981682089
C 0.2286178102 1.0977797108 -2.3845775989
C 3.5728802353 1.9803833664 -0.9156715302
C 0.934779565 3.5253622104 -1.7166206948
C -1.0873573329 1.4078759581 -3.041571829
C 0.299977831 -1.438648767 -2.9730582108
C 3.1974800067 -1.10571918 -1.7173536554
C 1.2794817513 -3.0826443683 1.5740629965
C 3.5268867468 -0.8269918379 2.0661005821
C 2.1736427128 1.64913826 3.4054041068
C -0.9260753101 0.938352476 3.9383171524
H 3.3757483547 2.7873960844 -0.1989880822
H 4.2322876021 1.2600705589 -0.4201859131
H 4.1582249454 2.4291830128 -1.7307173191
H -0.1229157534 3.8079632776 -1.6780711863
H 1.4162844408 3.959599549 -0.8321511372
H 1.3645564889 4.0403140925 -2.5874354582
H -1.4840403842 2.3794320844 -2.7298577591
H -0.9903899484 1.4475760475 -4.1354524868
H -1.856803414 0.6592231415 -2.8201974273
H 0.5832072624 -1.5382495829 -4.0307253388
H 0.6637523175 -2.3414551589 -2.4685215361
H -0.7948964417 -1.4646919405 -2.9386668066
H 3.9714769444 -0.8837545932 -0.9761677118
H 2.7810110358 -2.0888416798 -1.4673129945
H 3.7100374544 -1.2219807837 -2.6826777707
H 2.2451674991 -3.1949822376 1.0738774215
H 1.2382802237 -3.8372640356 2.3713135206

H 0.499122441 -3.3510709753 0.8517941441
H 3.7728433505 -1.6800107507 1.4294291261
H 3.9276956454 0.0713646861 1.584504969
H 4.0801602181 -0.9514333226 3.0063482459
H 1.4960128669 2.4417142098 3.7343725429
H 2.8492636355 1.4332219326 4.2431715687
H 2.7988967307 2.0600442797 2.6032593423
H -1.0907860066 0.5318297728 4.9456733546
H -0.6153893944 1.9800606362 4.0582576874
H -1.8964751953 0.9323744672 3.4307941171
C -1.1301832347 -2.1480986166 3.3733042518
H -2.0999014806 -1.6811491465 3.5729788904
H -1.3169133191 -3.0595210862 2.7969024696
H -0.6931793897 -2.4431763741 4.3345733447

I_Yb (lc)

E: -968.888604505 ; H: -968.325219 ; G: -968.430772
Yb 0.1605812489 0.3579389594 0.1033047684
H -3.2857372844 -1.8965360778 -1.0717339276
C -3.4140181117 -1.4498865579 -0.0787200086
C -2.3688905204 -0.4089187379 0.1637264884
C -2.4023800396 0.8456930394 0.4126406506
C -2.0386216454 2.1332985804 0.6333263888
H -4.4414069778 -1.0688816049 -0.0134310636
H -3.3186219867 -2.2775827228 0.6350418632
H -0.9570681507 -1.3401933349 1.9866454079
H -2.0665693773 2.5567710139 1.6359530857
H -2.046560871 2.850538163 -0.1857673445
C 0.0156986909 0.0725589073 3.2737376396
C -0.1810005813 -1.3422512675 2.7818759709
C 1.1683677557 -1.7214621349 2.2165882816
C 2.0310821121 -0.6834189505 2.4076711065
C 1.3073645091 0.4424611349 3.0483093195
C 0.829725774 -0.2098114847 -2.4843818582
C 2.0955715804 -0.1230700927 -1.8340054836
C 2.3012451521 1.2356859746 -1.4555522929
C 1.1633338849 1.9861489558 -1.872713145
C 0.2587050423 1.0948912605 -2.5166306613
C 3.5673599522 1.8291586394 -0.9022857716
C 1.0272411226 3.4801344129 -1.7767362726
C -1.026577039 1.4710796349 -3.1973079181
C 0.2539990805 -1.4361348603 -3.1364880088
C 3.0993724371 -1.2380993112 -1.7356568522
C 1.4494007249 -3.080378786 1.6588831958
C 3.502991564 -0.6445843893 2.1388021303
C 1.9762746007 1.7316701867 3.4177257154
C -1.0786373513 0.831059762 3.9496700808
H 3.3880962077 2.5607890822 -0.1030599514
H 4.2372136205 1.0623101918 -0.5001670747
H 4.1361280201 2.3604986812 -1.6785172516
H -0.0193345786 3.8000024446 -1.8000052992
H 1.4668291601 3.8813013244 -0.8555667039
H 1.5323065121 3.9895521312 -2.6099984443
H -1.4593330709 2.3862589655 -2.7804364178
H -0.8789808802 1.6513612824 -4.2714783443
H -1.7864709993 0.6878837427 -3.1060792056
H 0.5698494256 -1.5293499052 -4.1854605667
H 0.5670210133 -2.3594326599 -2.6349197707
H -0.8413137118 -1.4240967134 -3.1370634505
H 3.8039811303 -1.0929752523 -0.9098500925
H 2.623405998 -2.2147990904 -1.5876104686
H 3.7026046799 -1.3238968663 -2.6506684953
H 2.4118084368 -3.1207898252 1.143125126
H 1.4684703296 -3.8394425048 2.4522439015
H 0.6759181468 -3.3934243528 0.9474343111
H 3.8423631751 -1.5264486707 1.591637951
H 3.7933399505 0.2405594792 1.5644810854

H 4.0600284696 -0.6066033316 3.0835325778
H 1.262547725 2.4630762997 3.8032420869
H 2.7353495808 1.5697181318 4.1929903423
H 2.4948605407 2.1866502673 2.5655027779
H -1.2900800722 0.4123590568 4.9426286857
H -0.8258429894 1.8850551473 4.0870699548
H -2.008597898 0.7762640395 3.3735966245
C -0.6650140272 -2.3068867475 3.8775217517
H -1.6341831395 -1.9897757605 4.2725198363
H -0.7828754292 -3.3193913055 3.480778651
H 0.0517582181 -2.3414912631 4.7042730387

TS_{L,P}_Yb (lc)

E: -968.874124786 ; H: -968.315711 ; G: -968.417603
Yb 0.3896488678 0.3267738404 0.1976422313
H -3.4711726118 -1.9863000177 -0.4519114485
C -3.2358439974 -1.0942147639 -1.0437579644
C -2.5351753401 -0.0980895346 -0.2300673368
C -2.2496213423 0.9010957612 0.4318261206
C -1.6277503191 1.8820923866 1.2485161678
H -2.6320060472 -1.4228479342 -1.8960062451
H -4.1799155804 -0.6993376464 -1.4387194579
C 1.5410038955 0.5298841863 2.8278633759
C 0.0916577912 0.3541693895 3.042809599
C -0.1780284509 -1.0584629765 2.7116858291
C 0.993295729 -1.6384436225 2.2486754237
C 2.06654431 -0.6553827635 2.3362803388
C 0.8257904981 0.1510911663 -2.5168119737
C 2.1103285937 -0.0539679421 -1.9331291408
C 2.5247895927 1.1743109854 -1.3415930025
C 1.4918582219 2.1343455036 -1.5538224243
C 0.4466036284 1.5051215898 -2.2884108624
C 3.881945546 1.4737800324 -0.7691341123
C 1.5638994208 3.592307005 -1.1920064003
C -0.77771098 2.1858860208 -2.8319250888
C 0.0848583815 -0.8466101673 -3.3630750243
C 2.937765826 -1.3007745494 -2.078820985
C -1.4974063222 -1.7261070572 2.9540281446
C 1.1978319802 -3.0594801021 1.8073463437
C 3.5030077438 -0.9688035488 2.0395189517
C 2.2732021393 1.7937706249 3.1622591279
H 3.8372489759 2.1733347573 0.0739650629
H 4.3901030908 0.5712250725 -0.4161520422
H 4.5411352245 1.9331169099 -1.5193906886
H 0.5698982258 4.0342292665 -1.0607595864
H 2.1208944502 3.7643137535 -0.2635190461
H 2.0674910293 4.1824734742 -1.9708918845
H -1.1317769426 2.9894475515 -2.1767291736
H -0.5851944838 2.6416929729 -3.8134150437
H -1.6137950648 1.4914801835 -2.9612255099
H 0.4740832354 -0.8780771531 -4.3907341693
H 0.1590554559 -1.8707733082 -2.975664064
H -0.9795656324 -0.6025741931 -3.4424380296
H 3.7015290226 -1.3864211372 -1.2983962968
H 2.3300961509 -2.2133365887 -2.0408791504
H 3.4709970059 -1.3254807316 -3.0398879636
H -1.5820240929 -2.6749754775 2.4167473968
H -1.6318666134 -1.9476818662 4.0219396885
H -2.3363509891 -1.095067526 2.645288169
H 0.2478011847 -3.5772529639 1.6488350118
H 1.772889449 -3.1307650756 0.8761468974
H 1.7557169987 -3.632331277 2.559559135
H 4.1238741746 -0.070220391 2.0313653811
H 3.9150250334 -1.6448202958 2.8001743919
H 3.632939876 -1.4682527097 1.0732127291
H 2.3634291306 1.925519308 4.2490260785
H 3.2858157451 1.8043920867 2.7501316031

H 1.7521193784 2.6822500343 2.7847962929
C -0.5465502826 0.9592026711 4.2893225703
H -0.3605462138 2.0367226836 4.3446254128
H -1.631629236 0.8152854146 4.2843319117
H -0.1503294649 0.4998382206 5.2021527069
H -1.3269976809 2.7904043487 0.7152351809
H -2.2055422865 2.1498834729 2.136189288
H -0.5737794483 1.0943309959 2.1680855234

P_Yb (lc)

E: -968.921306007 ; H: -968.357269 ; G: -968.464421
C 2.6290232899 1.15971196 -0.830685863
C 2.7242016444 1.25033553 0.3771365675
Yb -0.1202003215 -0.0427796653 0.0420044511
C -1.0377481907 2.4993295383 0.697218125
C -1.0675551136 2.4609809425 -0.7268418779
C -2.0277884132 1.5979643343 1.1836324463
C -2.075419172 1.5344276203 -1.1216677574
C -2.6742015445 1.0064831534 0.0593992835
C 1.4105330927 -2.3834359939 0.0592200028
C 0.7018224243 -2.3766117428 1.2952886604
C 0.4603063701 -2.5510364571 -0.9890191535
C -0.6839463238 -2.5575544828 1.0121356489
C -0.8328533731 -2.6670160983 -0.4000660812
C -1.7613740435 -2.7609827824 2.0402970925
H -1.598445786 -2.1574524268 2.9409233873
H -2.7534669487 -2.5053581231 1.6547076561
H -1.8118065675 -3.8079616083 2.3717894497
C -2.0943186627 -3.0157691027 -1.1389599119
H -2.1659360228 -4.0968381248 -1.3252268907
H -2.9905646879 -2.7315351788 -0.579892232
H -2.1552118128 -2.5273320418 -2.1188196184
C 0.7696566286 -2.7506884143 -2.447501815
H 0.0160932883 -2.2985730695 -3.1040376409
H 1.74192726 -2.3280283721 -2.7254144459
H 0.8106519773 -3.8164041825 -2.7139882854
C 2.9049758213 -2.3991906543 -0.0995279101
H 3.3023318138 -3.4234254647 -0.0649750501
H 3.2286646444 -1.9700607519 -1.0540494016
H 3.4164732806 -1.8367136401 0.6886997957
C 1.3128923897 -2.363133049 2.6699084081
H 1.399824829 -3.3764157369 3.0870537978
H 2.3261637907 -1.9460979451 2.6650555523
H 0.7232138665 -1.7840609491 3.3917384698
C -3.8972181219 0.1354980275 0.1109518082
H -3.9877059083 -0.5046139288 -0.7722632036
H -3.9062188233 -0.5186880825 0.9893259719
H -4.8157553757 0.7377159489 0.1591864713
C -2.4296108193 1.4145445703 2.621367838
H -3.2199288995 2.1188271197 2.9175670264
H -2.8177647864 0.4088593757 2.8167739126
H -1.5941938022 1.5778596991 3.3122961604
C -0.2324907518 3.4595989608 1.5267721433
H -0.7483372455 4.4228872293 1.6483549203
H -0.0499195552 3.0814788654 2.5399294955
H 0.7405289551 3.6845088708 1.0744627151
C -0.2991758903 3.3761645452 -1.6382688034
H 0.7178646564 3.5702451549 -1.27685044
H -0.219174347 2.9735372244 -2.6548322285
H -0.7886250926 4.3557742703 -1.7352291217
C -2.5326349549 1.2692909735 -2.529982899
H -1.726417036 1.3987266415 -3.2614912408
H -2.9194520545 0.251718255 -2.6543295577
H -3.3400974919 1.9504156102 -2.8336363336
C 2.9328728409 1.3779914324 1.8164878115
H 2.22406131 2.0809646585 2.2643281109
H 2.8312730501 0.4132689938 2.3243017488

H 3.9430600392 1.7511005256 2.0162676958
C 2.6033966675 1.0709549517 -2.2877302134
H 2.3112592348 0.071319092 -2.6267396411
H 1.9106778056 1.7996063039 -2.7193550846
H 3.6000019619 1.2754836905 -2.6933209224

(Me₅C₅)₂Yb (sc singlet)

E: -1939.63788522 ; H: -1939.168543 ; G: -1939.254203

Yb 0.0183091041 0.2668609077 -0.8865684033
C 2.4532932451 0.9054892678 -0.0392304422
C 2.3798453001 -0.516336694 0.0445393459
C 2.3000450882 -1.032213485 -1.2825729879
C 2.3256101514 0.0705068976 -2.1865841944
C 2.4198895937 1.2681903157 -1.4181154071
C -2.2890812642 0.4628149167 0.4133399846
C -2.263784995 1.5653827711 -0.4908646613
C -2.3434050902 1.0492472382 -1.8178883665
C -2.4164854315 -0.3725829305 -1.7338681852
C -2.383027754 -0.7350292591 -0.3549192243
C 2.5925726249 2.6578673796 -1.9671401252
H 2.1947988904 3.4225301632 -1.2905528248
H 3.6517132223 2.9024532447 -2.1279029088
H 2.0922659495 2.7878395742 -2.933344665
C 2.6677986719 1.8464522778 1.1147005502
H 2.2455038309 2.8396158656 0.9245674958
H 2.2174946777 1.4747874158 2.0420117939
H 3.7362119213 1.9957645825 1.3236781404
C 2.5088045923 -1.3327548357 1.3012357803
H 2.1143572873 -0.8082069908 2.1786693486
H 1.9811207865 -2.2906388543 1.2313808864
H 3.558246563 -1.5700416671 1.5245734572
C 2.3253180254 -2.4864685937 -1.6661090908
H 3.3528102098 -2.8581662183 -1.7830599716
H 1.8473891273 -3.1227980924 -0.9127835781
H 1.8161266386 -2.6726059194 -2.6183488721
C 2.3877994734 -0.0221416451 -3.6866253439
H 1.9749269329 0.8678355768 -4.1742644847
H 3.4221511417 -0.1229976827 -4.0435644683
H 1.8387947479 -0.8881620473 -4.0734350935
C -2.5553651916 -2.1246449112 0.1943676624
H -2.1574704555 -2.8893349872 -0.4821147593
H -2.0549539421 -2.2543310503 1.1605564803
H -3.6144401519 -2.369433536 0.3552554391
C -2.6307246899 -1.3137977153 -2.8876426544
H -2.1804233725 -0.9422178379 -3.8149894578
H -2.2082520751 -2.3068429166 -2.6972949817
H -3.6990945733 -1.4633493495 -3.0966704229
C -2.472537274 1.8654049292 -3.0747370765
H -3.5220363288 2.1023489456 -3.2981703938
H -1.9451349025 2.8234548591 -3.0050257371
H -2.0778946484 1.3408165766 -3.9520588465
C -2.3513546763 0.5556898261 1.9133639972
H -3.385777511 0.6559480926 2.2702652776
H -1.9379195393 -0.3339285817 2.4011853519
H -1.8029144186 1.4221358477 2.3000165035
C -2.2894320838 3.0197032565 -0.1075996879
H -1.7803314743 3.2061453239 0.8446295544
H -1.8116247851 3.6560106686 -0.8610220547
H -3.3170191389 3.3911750603 0.0092332822

A₁Yb (sc singlet)

E: -2095.56346483 ; H: -2094.999565 ; G: -2095.102870

Yb -2.5781057684 -1.505494661 2.5647029657
C -3.3175816241 0.8552606512 3.622205464
C -3.4462489957 1.0310421482 2.2145364581
C -4.2974960011 -0.0920779952 4.0399974716
C -4.4949415821 0.1804847537 1.7597913749

C -5.0301759304 -0.5037249074 2.8889696539
C -0.9739950439 -3.6713187264 2.5672469982
C -1.5882833527 -3.6335383536 3.8521184849
C -1.9872477197 -3.9426374771 1.6033206793
C -2.9791925133 -3.8977693483 3.6836033873
C -3.2254667289 -4.0857073515 2.2926962187
C -3.9635757739 -4.1405147091 4.7920516493
H -3.7264906937 -3.5625143574 5.6910903613
H -4.9874529046 -3.8838175013 4.501563632
H -3.9765268091 -5.1982599473 5.0911462986
C -4.5203966444 -4.536175317 1.6769003271
H -4.5715647183 -5.6315892146 1.6001044072
H -5.3865375983 -4.2187350072 2.2647979807
H -4.6573729608 -4.1455580771 0.6618009573
C -1.7614773486 -4.2213833623 0.1431389789
H -2.6171015051 -3.9252874528 -0.4759536806
H -0.879181755 -3.7000137103 -0.2432905924
H -1.6013018611 -5.2925362993 -0.0449224552
C 0.5034563335 -3.6324605621 2.2968381319
H 1.0503744571 -3.0817279826 3.0709856668
H 0.935845767 -4.6426715556 2.2763063824
H 0.7416353415 -3.171035907 1.3316189631
C -0.8745037454 -3.4980637943 5.1694433043
H -0.5423237748 -4.4717481034 5.5562247111
H 0.0214282571 -2.8706269183 5.096240642
H -1.5148010746 -3.0570534195 5.9413069103
C -6.2718715114 -1.3490907486 2.8898345135
H -6.4032890886 -1.8950892214 1.9498558317
H -6.2693178924 -2.0876865255 3.6976107039
H -7.1733021841 -0.7350902638 3.0271436332
C -4.6160218875 -0.4493561234 5.4646535619
H -5.3256820821 0.2613192932 5.9116652154
H -5.0667461708 -1.4426719552 5.5470094444
H -3.7251140629 -0.4442741799 6.1030857954
C -2.4288726197 1.6469735361 4.5422598012
H -2.9424161708 2.5330573045 4.9408335127
H -2.1007154762 1.0622096277 5.4094940143
H -1.5257460917 2.013871501 4.0409366913
C -2.7542182445 2.0727564916 1.3804295729
H -1.8600471632 2.4683314858 1.8739395999
H -2.4438481972 1.697757581 0.3984937017
H -3.409984287 2.9349743384 1.1962189632
C -5.0459130873 0.1436085074 0.3609182562
H -4.2748505537 0.3479221222 -0.3910348684
H -5.4914445427 -0.8273565389 0.1169722372
H -5.833731852 0.895731828 0.2114815178
C -0.3754884876 -0.4494248612 0.5518439853
C -0.6592416253 -0.6776448123 -0.7050304947
H -1.5449423083 -1.2677421771 -0.9418547522
C 0.160602979 -0.1801748605 -1.8654261862
H 1.0283158235 0.3896515768 -1.5272069732
H 0.5108708023 -1.0209073477 -2.4744192732
H -0.4455598366 0.461658357 -2.5143674649
C -0.0511361963 -0.1968863317 1.8009779431
H -0.3845123491 0.7148404967 2.2935842325
H 0.621917636 -0.8551556342 2.3472955515

TS_{A-L}Yb (sc singlet)

E: -2095.52253625 ; H: -2094.963764 ; G: -2095.062019

Yb 0.3600409071 0.3899111083 0.2745405354
H -2.6924264664 -2.4244183769 -0.3923225792
C -3.1451629633 -1.7013524857 0.295520146
C -2.1851148128 -0.5912605197 0.6089372589
C -2.3333508479 0.6889633079 0.524958184
C -2.1770779363 2.017290539 0.515216103
H -4.0776263077 -1.3438037813 -0.1548587488
H -3.4007682402 -2.2580588988 1.2042676154

H -1.0482356203 -0.9566185212 1.5944442217
H -2.4631124058 2.6257169 1.3703453501
H -1.9349008551 2.5450643995 -0.4048948368
C 0.0880743103 0.1258711515 3.1938076064
C -0.2071971755 -1.1972212094 2.6172008958
C 1.0870471492 -1.7015808086 2.1236924626
C 2.0537889776 -0.728422222 2.3321349789
C 1.4272117657 0.4166908328 2.9817250032
C 0.8533973112 -0.1816515392 -2.3610917508
C 2.145263255 -0.0338788046 -1.7780549201
C 2.3126125352 1.3374564516 -1.4256214642
C 1.1259634588 2.0359891694 -1.7981682089
C 0.2286178102 1.0977797108 -2.3845775989
C 3.5728802353 1.9803833664 -0.9156715302
C 0.934779565 3.5253622104 -1.7166206948
C -1.0873573329 1.4078759581 -3.041571829
C 0.299977831 -1.438648767 -2.9730582108
C 3.1974800067 -1.10571918 -1.7173536554
C 1.2794817513 -3.0826443683 1.5740629965
C 3.5268867468 -0.8269918379 2.0661005821
C 2.1736427128 1.64913826 3.4054041068
C -0.9260753101 0.938352476 3.9383171524
H 3.3757483547 2.7873960844 -0.1989880822
H 4.2322876021 1.2600705589 -0.4201859131
H 4.1582249454 2.4291830128 -1.7307173191
H -0.1229157534 3.8079632776 -1.6780711863
H 1.4162844408 3.95959549 -0.8321511372
H 1.3645564889 4.0403140925 -2.5874354582
H -1.4840403842 2.3794320844 -2.7298577591
H -0.9903899484 1.4475760475 -4.1354524868
H -1.856803414 0.6592231415 -2.8201974273
H 0.5832072624 -1.5382495829 -4.0307253388
H 0.6637523175 -2.3414551589 -2.4685215361
H -0.7948964417 -1.4646919405 -2.9386668066
H 3.9714769444 -0.8837545932 -0.9761677118
H 2.7810110358 -2.0888416798 -1.4673129945
H 3.7100374544 -1.2219807837 -2.6826777707
H 2.2451674991 -3.1949822376 1.0738774215
H 1.2382802237 -3.8372640356 2.3713135206
H 0.499122441 -3.3510709753 0.8517941441
H 3.7728433505 -1.6800107507 1.4294291261
H 3.9276956454 0.0713646861 1.584504969
H 4.0801602181 -0.9514333226 3.0063482459
H 1.4960128669 2.4417142098 3.7343725429
H 2.8492636355 1.4332219326 4.2431715687
H 2.7988967307 2.0600442797 2.6032593423
H -1.0907860066 0.5318297728 4.9456733546
H -0.6153893944 1.9800606362 4.0582576874
H -1.8964751953 0.9323744672 3.4307941171
C -1.1301832347 -2.1480986166 3.3733042518
H -2.0999014806 -1.6811491465 3.5729788904
H -1.3169133191 -3.0595210862 2.7969024696
H -0.6931793897 -2.4431763741 4.3345733447

I_Yb (sc singlet)

E: -2095.53268640 ; H: -2094.969081 ; G: -2095.072576
Yb 0.1930783076 0.3307306913 0.1753550201
H -3.1814115271 -1.8395887244 -1.1533164437
C -3.3261970179 -1.39806776 -0.1602529221
C -2.2771666739 -0.3713475407 0.1115244624
C -2.2753415642 0.8803777476 0.3680644722
C -1.851263717 2.1459695973 0.607495499
H -4.3508974195 -1.0075799758 -0.1143622457
H -3.2548575965 -2.2320702352 0.5492830864
H -0.9078057782 -1.3341223436 1.8364229229
H -1.8830466261 2.5621909824 1.6129256769
H -1.8149629184 2.8707410315 -0.2034904747

C -0.0080050205 0.0931634404 3.162553198
C -0.1460905843 -1.320990761 2.6501690955
C 1.227730588 -1.6489422473 2.1148161383
C 2.0536901146 -0.5862513025 2.3459405786
C 1.2790022997 0.5068046915 2.9751031425
C 0.7348837183 -0.2611955408 -2.356647396
C 2.0145135772 -0.2045559503 -1.7330586421
C 2.2594749997 1.1491860792 -1.3589858898
C 1.1325636419 1.9258045432 -1.7569440934
C 0.1954877489 1.0563503871 -2.3809200167
C 3.5575470097 1.7194356586 -0.8586173557
C 1.0433676826 3.4232799886 -1.6650256846
C -1.0924661823 1.4542111127 -3.0428102725
C 0.1140562243 -1.4692130327 -3.0002121133
C 3.0000830766 -1.3372097708 -1.6734570646
C 1.5728464797 -2.9978374632 1.5687128092
C 3.5354765386 -0.5148324829 2.1515802303
C 1.8935066862 1.8125306909 3.3782404164
C -1.137829234 0.8016480179 3.8344373574
H 3.4225578324 2.4552498599 -0.0546823503
H 4.2284040364 0.9412498166 -0.4821268504
H 4.1026148894 2.2398250608 -1.6589651994
H 0.0078941338 3.7757105235 -1.6940619747
H 1.4889110604 3.8102887936 -0.7409136671
H 1.570595643 3.9133604688 -2.4960173472
H -1.4165922011 2.4523438616 -2.7327414649
H -0.9932448219 1.477112634 -4.1369225482
H -1.9093139806 0.764345622 -2.8049461423
H 0.3931835946 -1.5572702433 -4.0600899444
H 0.4249658046 -2.4025709954 -2.5168430224
H -0.9798528971 -1.4324998751 -2.9619787206
H 3.721162316 -1.2181459304 -0.858105151
H 2.5083996721 -2.3067830418 -1.5345479768
H 3.5852443524 -1.4152877536 -2.6008673259
H 2.5473433141 -3.0018144826 1.0751705057
H 1.6036892532 -3.7529320298 2.3658020091
H 0.8289886185 -3.3421344866 0.8405525491
H 3.9075507623 -1.3380272005 1.5383404234
H 3.8449605686 0.4232897701 1.6833313838
H 4.0454642161 -0.5705965217 3.122170699
H 1.1446879428 2.5143770385 3.7515728741
H 2.6364966832 1.6668776774 4.1721783849
H 2.4167315932 2.2945231819 2.5444369247
H -1.3519514859 0.3530081448 4.8137552351
H -0.9200138758 1.8591297582 4.0013133269
H -2.0549304296 0.7317652541 3.2397440121
C -0.630192726 -2.3168523347 3.7180023721
H -1.6183499957 -2.0344187438 4.0915443989
H -0.7068702458 -3.3257930594 3.3028014416
H 0.0655783787 -2.343235966 4.5627583041

TS_{L-P}_Yb (sc singlet)

E: -2095.52040956 ; H: -2094.961387 ; G: -2095.060251
Yb 0.3741599011 0.2959283904 0.2255841989
H -3.1868819135 -2.2337322879 -0.3737266879
C -3.0266792033 -1.3656564002 -1.0235897019
C -2.377833537 -0.2774328879 -0.2877376833
C -2.1843285732 0.790264598 0.2987322758
C -1.633532527 1.8495445756 1.059606343
H -2.4205661387 -1.7029900339 -1.8702201096
H -4.0048382891 -1.0598059742 -1.414767734
C 1.5659861692 0.5538671144 2.6923367183
C 0.1134481154 0.4242322813 2.9182582477
C -0.1961314486 -0.9913952743 2.6330973614
C 0.9589245059 -1.6155796465 2.1828039261
C 2.0567793866 -0.6623176306 2.23774234
C 0.7714868862 0.1979000904 -2.4192117114

C 2.0520301389 -0.043893374 -1.8425367348
 C 2.4806686994 1.158013226 -1.208455552
 C 1.4589661786 2.1360821522 -1.3853055894
 C 0.4074318812 1.5457468397 -2.1420529007
 C 3.8513692438 1.4333549979 -0.6590051112
 C 1.5550001296 3.5803199732 -0.9783607364
 C -0.8057968541 2.2560531422 -2.6704343213
 C 0.0257633215 -0.7524384457 -3.3131717922
 C 2.8716863759 -1.2863648883 -2.0528664003
 C -1.5259052171 -1.617955969 2.9212410853
 C 1.1232251884 -3.0551978966 1.7879876979
 C 3.4854601497 -1.0362887483 1.979283005
 C 2.3366576411 1.7981307006 3.0124485231
 H 3.8277129287 2.098204349 0.2117780816
 H 4.3670347355 0.5170087579 -0.357859637
 H 4.4898785064 1.9227541196 -1.4082378801
 H 0.5694159759 4.0307218373 -0.8170157976
 H 2.1269550978 3.7112902241 -0.0527754247
 H 2.0562365212 4.1881497266 -1.7450540173
 H -1.0868495948 3.1095929785 -2.0443326477
 H -0.6351138008 2.6505522801 -3.6819005495
 H -1.6799613797 1.5992537651 -2.7221027181
 H 0.4299179698 -0.7491231581 -4.3356215419
 H 0.079387411 -1.7915894999 -2.9646757714
 H -1.0325579912 -0.4853462079 -3.3950433897
 H 3.648315157 -1.4047812504 -1.2901454212
 H 2.2606427193 -2.197119229 -2.0407161652
 H 3.3872961262 -1.2727626001 -3.0237978974
 H -1.6307730908 -2.5960456432 2.4434838366
 H -1.6572007634 -1.7718612605 4.00135717
 H -2.354676491 -0.991898384 2.5773373044
 H 0.1588977457 -3.5572090187 1.6730613313
 H 1.6706247476 -3.1693160579 0.8448312933
 H 1.6898594162 -3.6118149807 2.5458535756
 H 4.1418697607 -0.1638612719 1.973552626
 H 3.8499583259 -1.7153147372 2.7614389404
 H 3.6166898668 -1.5565250336 1.0246865115
 H 2.4196328554 1.9450917273 4.0980614049
 H 3.3525910514 1.7654931789 2.6112207072
 H 1.8516812598 2.6966213259 2.6121827916
 C -0.5037595717 1.0919843212 4.1430556421
 H -0.2883822174 2.1651349758 4.1581816521
 H -1.5921233602 0.9767243152 4.1487617623
 H -0.1146638342 0.6551479506 5.0697966288
 H -1.3827745928 2.7475858523 0.4880538832
 H -2.2159781921 2.1150243464 1.9449854641
 H -0.5507379291 1.1467620267 2.0202272656

P_Yb (sc singlet)

E: -2095.56646808 ; H: -2095.002967 ; G: -2095.105944
 C 2.524668 1.112212 -0.810412
 C 2.6153 1.201809 0.397956
 Yb -0.098326 -0.031464 0.039981
 C -0.983709 2.430163 0.691697
 C -1.015883 2.386784 -0.731474
 C -1.963328 1.520641 1.183112
 C -2.014912 1.448916 -1.121317
 C -2.607413 0.920859 0.062404
 C 1.399765 -2.288394 0.039479
 C 0.695405 -2.280312 1.277469
 C 0.444374 -2.446574 -1.004857
 C -0.692135 -2.456568 0.999799
 C -0.846853 -2.561018 -0.411281
 C -1.753791 -2.680363 2.039314
 H -1.635276 -2.020653 2.90676
 H -2.75954 -2.51555 1.64208
 H -1.728943 -3.709962 2.423776

C -2.100726 -2.927836 -1.15292
 H -2.108434 -3.993851 -1.421074
 H -2.997343 -2.743584 -0.555651
 H -2.214528 -2.369724 -2.089985
 C 0.742427 -2.659022 -2.463856
 H 0.01315 -2.167646 -3.119585
 H 1.735602 -2.287549 -2.739342
 H 0.727348 -3.725496 -2.73018
 C 2.893121 -2.323617 -0.12285
 H 3.275479 -3.353267 -0.085188
 H 3.219068 -1.901422 -1.079314
 H 3.412689 -1.763572 0.661406
 C 1.308904 -2.289974 2.651049
 H 1.348678 -3.305404 3.0702
 H 2.340392 -1.921434 2.640983
 H 0.747945 -1.682472 3.372488
 C -3.841084 0.066889 0.120032
 H -3.948994 -0.563875 -0.767034
 H -3.849487 -0.592772 0.993544
 H -4.748783 0.684096 0.182189
 C -2.369439 1.351053 2.621113
 H -3.151164 2.06763 2.910705
 H -2.769825 0.351402 2.820273
 H -1.532584 1.507709 3.311583
 C -0.200268 3.4129 1.51515
 H -0.736026 4.366784 1.624006
 H -0.016048 3.047492 2.532276
 H 0.769875 3.651188 1.063977
 C -0.270003 3.317023 -1.645707
 H 0.747242 3.523269 -1.2922
 H -0.195104 2.92005 -2.664544
 H -0.775484 4.289456 -1.731686
 C -2.478776 1.185708 -2.527451
 H -1.672747 1.305464 -3.260479
 H -2.87488 0.171604 -2.64685
 H -3.280354 1.874579 -2.8292
 C 2.833631 1.325897 1.836055
 H 2.267123 2.162433 2.254771
 H 2.544607 0.413649 2.368312
 H 3.895765 1.501867 2.038275
 C 2.519184 1.023412 -2.267453
 H 2.083754 0.080272 -2.614838
 H 1.954488 1.84745 -2.712575
 H 3.545002 1.06953 -2.648833

[(Me₅C₅)₂Yb]⁺ (sc doublet)

E: -1939.43020950 ; H: -1938.959439 ; G: -1939.046970
 Yb 3.7720580457 1.1215130812 -2.4610166526
 C 4.0400073428 3.446960258 -3.5582879324
 C 2.7642280417 2.9564748828 -3.9591130722
 C 3.9946000386 3.6635489426 -2.1472638134
 C 1.9228982661 2.8756867809 -2.7913559169
 C 2.6805407326 3.3130170472 -1.6769936838
 C 4.1008091813 -1.3228430975 -1.7303854034
 C 4.0090830101 -1.336161206 -3.1535194651
 C 5.2972050068 -0.6343368264 -1.3807518655
 C 5.1726575649 -0.6728730725 -3.6882673239
 C 5.9647800432 -0.2408062077 -2.5982207514
 C 0.4664443524 2.5051633801 -2.795988303
 H 0.1205418888 2.1667083227 -1.8150694807
 H -0.1503089346 3.3710674162 -3.0663809357
 H 0.2337143914 1.7196384788 -3.5227166589
 C 2.1836716511 3.4912069629 -0.2696121517
 H 1.8506787114 4.5232176231 -0.1052651547
 H 1.3294072621 2.8454782765 -0.0463004696
 H 2.9577612433 3.2917345162 0.4788454145
 C 5.0810241647 4.2784041235 -1.3147815805

H 6.077133224 4.0881519066 -1.7244460921
H 4.9598915271 5.3685110044 -1.2740525412
H 5.0677517962 3.9258504174 -0.2785863258
C 5.1755173128 3.8133451153 -4.4723094905
H 6.149026016 3.7255241258 -3.9812065746
H 5.2006194905 3.1910276234 -5.3715084893
H 5.0815990214 4.8531787628 -4.807925952
C 2.3199763923 2.6947185488 -5.3683201155
H 1.8538501104 3.5924740517 -5.7941657919
H 3.1546007503 2.4317106513 -6.0241390143
H 1.5729976495 1.897077054 -5.43325386
C 7.3241742905 0.3926569742 -2.6728166008
H 7.4868452428 0.9097525434 -3.6222039022
H 7.4980648749 1.1114023043 -1.8655607768
H 8.108130932 -0.3699993026 -2.5866791334
C 5.851944215 -0.4626090143 0.0035161094
H 5.0736346225 -0.493934679 0.7714391047
H 6.5563543912 -1.271127205 0.2368521768
H 6.4059020113 0.474452324 0.1214001805
C 3.1523428858 -1.9964975807 -0.776986367
H 3.4584200532 -3.0335074888 -0.5943206694
H 3.1195009771 -1.5029195345 0.1993099309
H 2.1292075489 -2.0358436921 -1.1637944696
C 2.9639556481 -2.0434322021 -3.9663297233
H 2.7779559045 -1.5550857668 -4.9281381452
H 3.2861458092 -3.0674548122 -4.1943823089
H 2.0090696877 -2.1265482887 -3.4387564905
C 5.5282376146 -0.5865954984 -5.1448744722
H 4.6478337858 -0.4697403175 -5.7846808247
H 6.2068348104 0.2442205346 -5.3560253015
H 6.0345883996 -1.5028912419 -5.472731869

A_Yb (sc triplet)

E: -2095.51968441 ; H: -2094.956376 ; G: -2095.054827
Yb 2.7626999658 1.1555588246 1.1191509168
C -0.599428353 -0.1074480224 0.6371635174
C 3.7620710184 -0.5718776693 -0.5568596604
C 4.8627629399 0.2345669665 -0.133705811
C 3.3309664996 -1.3544374045 0.5522818913
C 5.0896199955 -0.027306889 1.2477310411
C 4.1406455166 -1.007103102 1.6697366267
C 1.5233735718 3.3483032557 1.9183958485
C 2.8267203848 3.3838773875 2.4944453954
C 1.6639080912 3.4497129246 0.5089862352
C 3.7737663809 3.547288727 1.4402854435
C 3.054742388 3.5765359039 0.2082688661
C 0.5335757759 3.582560614 -0.4702407096
H 0.2145014106 4.6299152113 -0.5647629272
H 0.8134241701 3.2468526353 -1.4741087696
H -0.3389343717 3.0020298957 -0.1583134559
C 3.6149354762 3.9129937225 -1.1448093302
H 4.6901989968 3.7281524921 -1.2012208341
H 3.1408806747 3.339182974 -1.9492600169
H 3.4568100705 4.9738877775 -1.381229547
C 5.2276257399 3.8745840545 1.6245945441
H 5.6600821975 3.3717065848 2.4944455601
H 5.8297817306 3.599740924 0.7541613478
H 5.3665466448 4.9534099356 1.7784916379
C 3.1393737483 3.3833829882 3.9644510034
H 3.0757716017 4.3940258143 4.3894586295
H 2.4463427556 2.7529450664 4.5312604805
H 4.1514690427 3.0180757045 4.1666415363
C 0.2177362147 3.3651553451 2.6566747827
H -0.2447809189 4.3592691884 2.601179486
H -0.4995644274 2.6471983697 2.2448146496
H 0.3481686863 3.1359826938 3.718160033
C 2.313916409 -2.4564701999 0.5081808557

H 2.7935281838 -3.420203991 0.2894082662
H 1.7797770105 -2.5674287531 1.4561738135
H 1.5575293507 -2.2824326517 -0.2609564105
C 4.1369849345 -1.6728248635 3.0157883354
H 4.950781622 -2.4065918624 3.0930909
H 4.2736678211 -0.960590767 3.8372100913
H 3.2041913074 -2.2121726568 3.201338072
C 6.2564752579 0.4409594621 2.0699021378
H 7.0325957925 -0.334753584 2.1228603194
H 6.7249763412 1.3333627113 1.6481522064
H 5.9759614268 0.67298408 3.1035654985
C 5.7599966285 1.0187818733 -1.0465430928
H 5.2158711833 1.4595143838 -1.8868408028
H 6.2745684972 1.8305417868 -0.5249665086
H 6.5377621 0.3720942444 -1.4752545614
C 3.2504397626 -0.6843641194 -1.9656485131
H 2.202359602 -0.9965225773 -1.9935306911
H 3.3268667253 0.2623637872 -2.5114257894
H 3.821597597 -1.426486156 -2.5396950243
C 0.4808664408 0.1802166864 1.3562129546
C 1.0267445307 0.1345103097 2.6424965057
C -0.7834334082 0.0783992249 -0.8411373447
H -0.9707396089 -0.8825603686 -1.3387850193
H -1.6495550329 0.7151781318 -1.0632877762
H 0.0989254744 0.5332843088 -1.3010611904
H -1.4594612621 -0.5511504407 1.1554005099
H 1.4263285133 -0.8022994646 3.0290589064
H 0.7346141814 0.8672235715 3.3937199409

P_Yb (sc triplet)

E: -2095.52753894 ; H: -2094.962961 ; G: -2095.063577
C 2.220765068 0.9964215725 -0.8425994813
C 2.3125719819 1.0785367587 0.4278221053
Yb 0.0945153215 0.0439526545 0.0042989949
C -0.8502252029 2.4219358543 0.6934964325
C -0.8879775233 2.3990851322 -0.7290822013
C -1.8105626482 1.4821971561 1.1769140732
C -1.8684306149 1.441924213 -1.1295596636
C -2.4574676896 0.8951476555 0.0491354823
C 1.505917593 -2.2300040458 0.0242556769
C 0.7975547745 -2.1834498059 1.2581442017
C 0.5524561865 -2.3630621169 -1.0242051695
C -0.5963218463 -2.3294453778 0.9772380539
C -0.7474438549 -2.4432614902 -0.4363601369
C -1.6574001072 -2.5514720855 2.0169168434
H -1.5434111001 -1.8861705236 2.879451232
H -2.6637209757 -2.400936495 1.6178639799
H -1.6170231832 -3.5788028878 2.4038020607
C -1.9968810345 -2.819496379 -1.1799347416
H -1.9832295511 -3.8846292845 -1.4480698322
H -2.8951290428 -2.6513825635 -0.5819803414
H -2.1161375066 -2.2620882051 -2.115915285
C 0.8542405836 -2.5593729845 -2.4835514911
H 0.0936588073 -2.1066479554 -3.1293029967
H 1.8204920194 -2.1295319039 -2.7636167319
H 0.8918989136 -3.6263017787 -2.7430201855
C 2.9966707198 -2.2543668783 -0.133606054
H 3.3791425723 -3.2825142708 -0.0790431036
H 3.3140939945 -1.839531802 -1.0943096928
H 3.50185198 -1.6757761839 0.6446140564
C 1.4081247685 -2.1587917762 2.6314332463
H 1.5140402557 -3.1734937071 3.0391090706
H 2.406410773 -1.7119604218 2.6247153456
H 0.8014110339 -1.5947274318 3.3487151253
C -3.7058390244 0.064257082 0.0953878602
H -3.8287048663 -0.5517585089 -0.7989485457
H -3.73535405 -0.6004288666 0.9632538354

H -4.5925045885 0.7098909354 0.1609773264
C -2.2068653575 1.2969356846 2.6153919622
H -2.9356252889 2.05684109 2.9287467144
H -2.6689911132 0.3210192878 2.7910562896
H -1.3529561048 1.3820352135 3.2966756405
C -0.0561763674 3.381942628 1.5300508786
H -0.5949440114 4.3304030448 1.6623097785
H 0.1419912709 2.9879167983 2.5322012234
H 0.9084380985 3.6175942035 1.0710222854
C -0.1400967724 3.3320181173 -1.6351642146
H 0.867880555 3.539658778 -1.2635014445
H -0.0413054285 2.9281077817 -2.6476598203
H -0.661242043 4.2949276381 -1.726147664
C -2.3227692251 1.1901317349 -2.5405444195
H -1.5050045732 1.2917205443 -3.2622265806
H -2.7442979761 0.1876681077 -2.6643587046
H -3.1016689127 1.9026400293 -2.8441135957
C 3.18407099 1.4773904743 1.5680177123
H 2.6766665372 2.1770918294 2.2403780132
H 3.4672124373 0.6079755332 2.1724030519
H 4.1096666674 1.9566862982 1.2182425892
C 2.912569372 1.2491166879 -2.1375068199
H 3.0632900146 0.3185982243 -2.6963610968
H 2.32727759 1.9135961665 -2.7821450757
H 3.8983390008 1.7113202601 -1.9845354853

Ca

(Me₅C₅)₂Ca (large core)

E: -1457.59318753 ; H: -1457.121546 ; G: -1457.211337

C -3.2016094886 0.7171538233 3.441598005
C -3.2633320066 0.706611733 2.0170186604
C -4.4201887565 0.1692350837 3.9394626036
C -4.5201821049 0.1521969196 1.6343815949
C -5.2353369266 -0.1798259806 2.8226148234
C -1.1324804263 -3.4461289157 2.6688982027
C -1.8471771369 -3.7771714566 3.857674545
C -1.9484530363 -3.7952246573 1.5526471746
C -3.1045978928 -4.3309317184 3.4759510434
C -3.167112443 -4.342113987 2.0514178967
C -4.1306177257 -4.9150679834 4.4077478611
H -4.1295495494 -4.4229632828 5.3868119075
H -5.1474210847 -4.8386609102 4.0061476483
H -3.9469773217 -5.9821088632 4.5936721131
C -4.2720451254 -4.9365825968 1.222174938
H -4.1056538225 -6.0057243747 1.03221541
H -5.2484650955 -4.8547632829 1.7128686156
H -4.3592303872 -4.4549352396 0.2417698795
C -1.5441606973 -3.7140717322 0.1063001902
H -2.4054119053 -3.5813858504 -0.5581152588
H -0.854603931 -2.8842658591 -0.0855874655
H -1.0325346524 -4.6286577222 -0.223260255
C 0.2805484095 -2.9354686568 2.6013327768
H 0.5424756866 -2.3240130098 3.4720651048
H 1.0070771611 -3.7587098034 2.5664800332
H 0.4587499649 -2.3242033031 1.7093731693
C -1.319133636 -3.6736281053 5.2621942489
H -0.8064038628 -4.5947634024 5.5710062431
H -0.5933131618 -2.8601270772 5.3721461248
H -2.1161366261 -3.4994607449 5.9939714013
C -6.6481771518 -0.6911432215 2.8890021541
H -6.9090482323 -1.3028418904 2.0181216045
H -6.8268791034 -1.3023605279 3.7808871661
H -7.3750939399 0.1317858852 2.9230825369
C -4.8250154165 0.0871615593 5.3855997037
H -5.3359772523 1.001887885 5.7158132155
H -5.5153217771 -0.7422409875 5.5764797535
H -3.9640891034 -0.0468139214 6.0501889249
C -2.0978699662 1.312139003 4.2720643311
H -2.2678123366 2.3799238597 4.4664626214
H -2.0078177357 0.8269710756 5.250503783
H -1.1217680891 1.2356527476 3.7799404588
C -2.2371366715 1.2915290265 1.0858930091

H -1.220683971 1.2168674052 1.4886801344
H -2.2363743827 0.7986821979 0.107187684
H -2.4220989635 2.3581546193 0.8989146414
C -5.0473056072 0.0487373143 0.2295096107
H -4.2496229855 -0.123884595 -0.5018861302
H -5.7719356835 -0.7657083113 0.1186421482
H -5.5611487041 0.9693286712 -0.0790832814
Ca -3.1833373453 -1.8122968387 2.7458816943

A₂Ca (large core)

E: -1613.51402426 ; H: -1612.950023 ; G: -1613.052065

C 0.3828268456 -0.1325238613 2.0761371055
C 0.9840359694 0.2960163634 3.1563663708
C -3.3221755145 0.8012678185 3.5255582633
C -3.3396090626 0.9862733753 2.1125721436
C -4.3715415292 -0.1006484556 3.8652937257
C -4.3883022165 0.1839651013 1.5769242484
C -5.0322293082 -0.4802415606 2.6617345332
C -1.0344782167 -3.7228118761 2.5669692042
C -1.7291243611 -3.6950476491 3.8108537083
C -1.9894023614 -3.9572971704 1.5357820509
C -3.108876123 -3.9397789687 3.5521506756
C -3.271052664 -4.0942525571 2.1453955908
C -4.1685480681 -4.1662404711 4.5925655041
H -3.9823089241 -3.591538356 5.5058676365
H -5.1662450571 -3.892731841 4.2338360558
H -4.2181604321 -5.2233432032 4.8888677793
C -4.5340638085 -4.4973500138 1.4374316886
H -4.5993660864 -5.5880651159 1.3191482125
H -5.4284999663 -4.1831417743 1.9834578611
H -4.6019603515 -4.0699372857 0.4301734873
C -1.6972291506 -4.1881256211 0.0784557536
H -2.4936592332 -3.8056530747 -0.570943758
H -0.7631279674 -3.7132122472 -0.2424412368
H -1.5959602553 -5.2578432397 -0.1509702913
C 0.461277431 -3.7097225627 2.4155290005
H 0.944662777 -2.9038123611 2.9802687155
H 0.9023476415 -4.6514067944 2.7696199953
H 0.7673563336 -3.6027050343 1.3696462363
C -1.0856967519 -3.5886470788 5.1658798038
H -0.7771049561 -4.5714429289 5.5493180773
H -0.1836101391 -2.9658398923 5.1463901509
H -1.7630685102 -3.1603715014 5.9130786637
C -6.2930581866 -1.2910663672 2.5654510326
H -6.3653406032 -1.8359262435 1.6184476876
H -6.373790817 -2.0272229895 3.3717700649
H -7.1849725307 -0.6522111727 2.6310018123
C -4.8002586626 -0.4575645304 5.260714957
H -5.5083640749 0.2788587722 5.6656644025
H -5.2968164783 -1.4317411822 5.3026894806
H -3.9547614749 -0.4944443553 5.957245265
C -2.4691051264 1.5633054532 4.5015116523
H -2.9703311349 2.4772833308 4.8498769747
H -2.23636377 0.9780164993 5.3993981791
H -1.5185873207 1.8776027567 4.0569120616
C -2.5347436397 2.0049816574 1.3558097622
H -1.5093270121 2.0972609676 1.7317450325
H -2.476769206 1.772441401 0.2863278749
H -2.9869645827 3.0037835588 1.4284613453
C -4.836401076 0.1532795802 0.141346198
H -4.0108814019 0.3345261006 -0.556755346
H -5.2833710804 -0.8099471205 -0.1294476174
H -5.5952450199 0.9204192243 -0.0663374958
C 2.3622769362 0.9000470865 3.1831245468
H 2.3268187825 1.9165854454 3.5905443162
H 3.0245384298 0.3134212216 3.8296451342
H 2.8006125474 0.9413138332 2.1840029387
C -0.1948602057 -0.5572894444 0.9749740079
H -0.0405799985 -1.5730126131 0.6167383856
H -0.7820603221 0.1173079664 0.3546818229
H 0.4584329158 0.2162878802 4.1083538298
Ca -2.6125828696 -1.5561628785 2.5146157379

TS_{A-L}Ca (large core)

E: -1613.46966159 ; H: -1612.910836 ; G: -1613.009448

H -2.6746313964 -2.2565277518 -0.6332384071

C -3.1000429269 -1.5981314386 0.1327341385
C -2.125485634 -0.5215159301 0.5048219565
C -2.235527463 0.7636208547 0.498805877
C -2.0202599043 2.0807699995 0.5818392517
H -4.0473889461 -1.2016449092 -0.2492843786
H -3.3231301164 -2.234056362 0.9969810965
H -1.0026803537 -0.9425464865 1.4952215051
H -2.2749568865 2.6378642779 1.4807633107
H -1.7587001524 2.6632097484 -0.29862045
C 0.0934006486 0.1445498345 3.1037142486
C -0.1820010348 -1.1816520873 2.5203343041
C 1.1226935269 -1.6725185862 2.0417824781
C 2.076252484 -0.6900521318 2.2627435386
C 1.4309258642 0.4494458506 2.9022217365
C 0.7994217377 -0.2436126488 -2.2355196412
C 2.0942492073 -0.0857377833 -1.663662844
C 2.2572579122 1.2882204753 -1.3221630918
C 1.0666601151 1.9790923813 -1.6964056401
C 0.1705277762 1.0336158935 -2.2707871748
C 3.5188988165 -1.1512010416 -0.8479666631
C 0.8859426054 3.4702985856 -1.6300590236
C -1.1533493629 1.3255067852 -2.91908666016
C 0.2493431667 -1.5079652095 -2.8341729782
C 3.1528459705 -1.1512010416 -1.6207576749
C 1.3347681592 -3.0521309036 1.4969966409
C 3.5550485435 -0.7805318297 2.034320715
C 2.1582707797 1.6922165348 3.3263590395
C -0.9315094353 0.9373917506 3.8538416343
H 3.3278214725 2.7432822644 -0.1101257411
H 4.2151901667 1.242638452 -0.3933581201
H 4.0574727096 2.43214976 -1.6782686545
H -0.1641460079 3.7638225458 -1.7249639074
H 1.2566029961 3.8978089425 -0.690008576
H 1.4289065272 3.9791541491 -2.4385514862
H -1.510005997 2.332923357 -2.6847766941
H -1.0837476725 1.2633206365 -4.0134335276
H -1.9370216836 0.6258383903 -2.6070914301
H 0.5465729502 -1.6235697815 -3.8862157269
H 0.6036559961 -2.4033258562 -2.310131168
H -0.8456403053 -1.527299444 -2.8126642438
H 3.9689855412 -0.8933179619 -0.9399738199
H 2.7575200898 -2.1234938078 -1.3041932302
H 3.6028965852 -1.3045389258 -2.6114029245
H 2.3138057212 -3.1593872337 1.0230167561
H 1.2745507539 -3.806633606 2.2930722323
H 0.5752975098 -3.3216961741 0.7532296423
H 3.8218616522 -1.6360760233 1.4103125785
H 3.9602382806 0.1182608199 1.5586846499
H 4.0822608977 -0.8964581067 2.9903796947
H 1.4678263355 2.4830319511 3.6320845196
H 2.8200518458 1.4926618812 4.1790065401
H 2.7924549081 2.095263332 2.5278568089
H -1.0664047573 0.5371803036 4.8681854406
H -0.6482736923 1.9886217629 3.9559246471
H -1.9089166626 0.8969647265 3.3621197328
C -1.1061177307 -2.1438222398 3.2607132059
H -2.0830623725 -1.6872610473 3.4474856625
H -1.2742623416 -3.0551913547 2.6787381552
H -0.6789964874 -2.4361879517 4.2271060361
Ca 0.3566770704 0.3705722681 0.2957190452

I_Ca (large core)

E: -1613.48103036 ; H: -1612.917096 ; G: -1613.019662
Ca 0.2083741262 0.4170198917 0.0705804122
H -3.2985636023 -1.5719615776 -1.0829974688
C -3.3482313832 -1.1830645291 -0.0589837577
C -2.254174895 -0.1952653546 0.1749004172
C -2.1939800502 1.0486110713 0.4573619947
C -1.7014505337 2.2896579225 0.7003355239
H -4.3541958429 -0.7708358953 0.0930864179
H -3.2416711762 -2.0560306402 0.5972743455
H -0.9512452631 -1.4495189149 1.9300422764
H -1.6490480833 2.6761474834 1.7170284577
H -1.6861443926 3.0367109128 -0.0912832692
C -0.0568815442 -0.0127227876 3.2375502299
C -0.1820815166 -1.429145951 2.7257555769

C 1.1857451521 -1.7323370843 2.1573998504
C 1.9951189831 -0.6567990463 2.3683125013
C 1.2130264396 0.4250887447 3.017726714
C 0.7918709493 -0.273038508 -2.4059366668
C 2.0593488819 -0.1614742747 -1.7631232531
C 2.2657465385 1.2119018708 -1.4375342689
C 1.1283676567 1.9449699882 -1.8842138209
C 0.2213008934 1.0295036099 -2.4877445598
C 3.5346064823 1.8308018183 -0.9193221119
C 0.9957359334 3.4414548072 -1.8564120021
C -1.0666429115 1.3863279374 -3.1736994531
C 0.2119978485 -1.5259121709 -3.0008281634
C 3.0706840085 -1.2666955382 -1.6400705521
C 1.5380666159 -3.0705442177 1.5915840528
C 3.4682710429 -0.5459197274 2.1285692218
C 1.8149381415 1.7453187975 3.3920513622
C -1.1929246068 0.6872622981 3.9053448632
H 3.3593811279 2.5742586254 -0.1303340544
H 4.2215105855 1.0795914601 -0.5174192561
H 4.0792116919 2.3546676676 -1.7171036817
H -0.0502674419 3.761329213 -1.8948173911
H 1.4372491679 3.8822466125 -0.9549333939
H 1.5018339841 3.9069973698 -2.7140469289
H -1.562188059 2.2413931044 -2.701774358
H -0.902237177 1.6524619546 -4.22712879
H -1.7802057949 0.556744183 -3.1591152239
H 0.4905811042 -1.6436730414 -4.0573930835
H 0.560286116 -2.4273663141 -2.4837901784
H -0.8825073043 -1.5309658381 -2.9588343694
H 3.7744609821 -1.0974471584 -0.8187154136
H 2.600849495 -2.2422938533 -1.4709508727
H 3.6722717884 -1.3657630953 -2.5545546115
H 2.5180247382 -3.0661549001 1.1088802744
H 1.5594325615 -3.8396746389 2.3751059157
H 0.8019175804 -3.4016223074 0.8493250382
H 3.8639248026 -1.4154151385 1.6000776314
H 3.7263859159 0.3470743675 1.5512662068
H 4.0007418737 -0.469932533 3.0851075294
H 1.0694434828 2.4293103498 3.8029229096
H 2.602057951 1.618816904 4.1454964818
H 2.2833437034 2.2408591226 2.5330442836
H -1.4652052756 0.186081245 4.8432786142
H -0.9529826985 1.7252637048 4.1472432314
H -2.0823710331 0.6826724713 3.2651526822
C -0.6076401107 -2.4317353848 3.8115635216
H -1.5896287999 -2.1714066659 4.2165752462
H -0.6745877892 -3.444437444 3.4033898382
H 0.1150289395 -2.4386789785 4.6339193325

TS_{1-p}_Ca (large core)

E: -1613.46734956 ; H: -1612.908160 ; G: -1613.006415
H -3.2570195678 -2.103876522 -0.3191053893
C -3.0951700345 -1.2347458164 -0.9674441066
C -2.4269883892 -0.1560316045 -0.2378464477
C -2.1651207975 0.8959090825 0.3465874556
C -1.5538978265 1.9279806862 1.1028321439
H -2.5019057851 -1.5746290146 -1.822421539
H -4.074324871 -0.9175415974 -1.3468665048
C 1.5655799353 0.5339579513 2.7393624934
C 0.1102149987 0.3915814919 2.9354035193
C -0.1890724942 -1.0146523998 2.5932999685
C 0.9747971512 -1.6167983445 2.1390974684
C 2.0685237431 -0.6598806902 2.2473781863
C 0.7791229779 0.1534619809 -2.4025588773
C 2.0631332907 -0.052998793 -1.8189753433
C 2.478946168 1.1752877641 -1.2286537559
C 1.4472439646 2.1356174508 -1.4409581536
C 0.4023179426 1.5076208965 -2.1768878599
C 3.8370051194 1.4809308593 -0.6642543705
C 1.5274125439 3.5942001107 -1.085417218
C -0.8192564909 2.1879985847 -2.7254529701
C 0.0425478944 -0.8443012904 -3.2515502973
C 2.890740983 -1.2968905748 -1.9848646095
C -1.5187247948 -1.6595633751 2.8393863736
C 1.1523795306 -3.0381497277 1.6895984947
C 3.5020665335 -1.0133815932 1.9880807024

C 2.3202952121 1.7786078123 3.0924510094
H 3.7895548016 2.1629371807 0.1924914247
H 4.3591371152 0.5782965789 -0.3346657776
H 4.4805964747 1.9641906351 -1.4127049087
H 0.536812975 4.0407618751 -0.945595901
H 2.0943657908 3.7655069022 -0.1630700474
H 2.025790809 4.1772111646 -1.8725491886
H -1.1232273222 3.042260503 -2.1114022084
H -0.6443328093 2.5731692613 -3.7395263626
H -1.6792855905 1.5134242819 -2.777718063
H 0.4807613256 -0.9219716885 -4.2565358636
H 0.0603251867 -1.8572578499 -2.8288036021
H -1.0059588457 -0.5618117441 -3.3884419509
H 3.7151904823 -1.343450165 -1.2663440016
H 2.3010447582 -2.2146752689 -1.8670885045
H 3.344318177 -1.3480282643 -2.984751198
H -1.6159864237 -2.6126004354 2.3115919974
H -1.6547060582 -1.8689784117 3.9094789384
H -2.3470249946 -1.0191392817 2.5221452764
H 0.1925556059 -3.5298505726 1.5095580562
H 1.7415648007 -3.1114092904 0.7680030758
H 1.6829633017 -3.6301990662 2.4466286668
H 4.1516431499 -0.1358589035 2.0132340171
H 3.866570824 -1.7118811081 2.7527003072
H 3.6433066539 -1.5047287661 1.0200614964
H 2.3971117975 1.9005864614 4.1813871252
H 3.3377881245 1.7692029039 2.6933234663
H 1.8231386035 2.6794413318 2.7123550208
C -0.5284492856 1.004954249 4.1780832713
H -0.3094693495 2.0754065832 4.2455127792
H -1.6170782025 0.8944947601 4.1556789853
H -0.1590908113 0.5247190869 5.0913683976
H -1.2564026055 2.807969181 0.5246836926
H -2.1253646804 2.2326588403 1.9827763548
H -0.5148434393 1.1524933381 2.0625780022
Ca 0.3914287234 0.3493583708 0.2156448533

P_Ca (large core)

E: -1613.51649839 ; H: -1612.951646 ; G: -1613.055903 ; D:
C 2.5686417405 1.1316974281 -0.8264429455
C 2.6739546336 1.2273967294 0.3799758387
C -0.9779853376 2.4020167091 0.7011145228
C -1.0138084393 2.3603746223 -0.7226345071
C -1.9711692995 1.5077704891 1.1934917447
C -2.0276265967 1.4377037474 -1.1107790104
C -2.6261867874 0.9186685367 0.0737634503
C 1.3807152661 -2.2654516901 0.0572235694
C 0.6627581498 -2.2654871494 1.2877312762
C 0.4385085496 -2.4352548014 -0.9977567775
C -0.7186997873 -2.4637750983 0.9946876548

Sm

(Me₃C₃)₂Sm (large core)

E: -808.905913146 ; H: -808.438096 ; G: -808.520308
C 4.191010306 -0.7099342091 -1.5596583388
C 5.4773571572 -0.2353842171 -1.1727762328
C 3.5164913919 -1.1585877456 -0.3875538657
C 5.5977792564 -0.3904803199 0.2382460198
C 4.3860912253 -0.9614488974 0.7236057806
C 1.8469871135 3.589917669 0.9982306497
C 3.1350486086 4.0622201512 1.3821585845
C 1.7241564639 3.7438865843 -0.4127086528
C 3.8082213274 4.5083311798 0.2083114966
C 2.9360702443 4.3118959149 -0.9009686214
C 0.4887886355 3.4682363529 -1.2252725094
H -0.1720528046 4.3449430531 -1.2753334895
H 0.7227663545 3.1990335956 -2.2620823303
H -0.1120231723 2.6526926679 -0.8057502939
C 3.2005339215 4.7398256793 -2.3185320868
H 4.2672326057 4.7111556589 -2.5701947813
H 2.6773990609 4.1105956819 -3.0484179822
H 2.8664886124 5.7703075092 -2.5036615051
C 5.1546458257 5.1773757323 0.1658924084
H 5.8249442577 4.8147914037 0.9542794856
H 5.6667565659 5.0235466636 -0.7912974538

C -0.856973981 -2.5699926965 -0.4173949265
C -1.7896793527 -2.6847601169 2.0251563794
H -1.72199923 -1.976476804 2.8594241283
H -2.7929755821 -2.5905147314 1.6000189063
H -1.7225158825 -3.6907847576 2.4623319604
C -2.1010242494 -2.9364109578 -1.1757362302
H -2.0971429702 -3.9985850256 -1.4577106172
H -3.0049870971 -2.7670260896 -0.584905033
H -2.2098460571 -2.3669192887 -2.1066614515
C 0.7543376579 -2.6395294408 -2.4540625901
H 0.027389773 -2.1524840713 -3.1159013767
H 1.7471038276 -2.2583702251 -2.7171728374
H 0.7514438322 -3.7050844489 -2.7233583826
C 2.8759314351 -2.2878282572 -0.0895604284
H 3.2623466364 -3.3159186857 -0.0559672802
H 3.2094860599 -1.8553988666 -1.0385833462
H 3.3832914082 -1.7320063872 0.7054010396
C 1.2571964251 -2.2578902671 2.66934308
H 1.3026052284 -3.269902355 3.095513084
H 2.2839739096 -1.8766935393 2.6714364112
H 0.6780073117 -1.6516094492 3.3772835659
C -3.8605079788 0.0654458706 0.1323902746
H -3.9666013687 -0.5691786125 -0.7523061972
H -3.8713287453 -0.5903812743 1.0087784179
H -4.7674147971 0.68389259 0.189287855
C -2.3710393438 1.3391173853 2.6332052113
H -3.1220050923 2.0825368084 2.9352793243
H -2.8089336019 0.3539804427 2.824935172
H -1.5234971359 1.4562992536 3.3186790958
C -0.1807945429 3.3735797897 1.5244661034
H -0.7058631086 4.3330148912 1.6345185726
H -0.0005744577 3.0046177784 2.5410914023
H 0.7913035051 3.6002938921 1.0720002685
C -0.2600767474 3.2830798968 -1.6379495636
H 0.7568380492 3.4846935962 -1.2815905976
H -0.1848984251 2.8826168173 -2.6553004954
H -0.761718203 4.2569986628 -1.7269237333
C -2.4928155233 1.1770436138 -2.5169044813
H -1.6843657219 1.2855925189 -3.249087929
H -2.9024523203 0.1681137114 -2.6349463572
H -3.2848953536 1.8759388141 -2.8198189716
C 2.9085682308 1.3546403587 1.8149213226
H 2.236233743 2.0882742704 2.2687134187
H 2.7706117685 0.398327346 2.3296598077
H 3.9370404035 1.6841533172 1.9976624298
C 2.5440666921 1.0322566535 -2.2825238407
H 2.0847085274 0.0961131193 -2.6174582882
H 1.9907313746 1.8637611574 -2.7281668768
H 3.5656166738 1.0548350707 -2.6769408094
Ca -0.1428126953 -0.0513118013 0.044939593

H 5.0760787145 6.2649376349 0.303194113
C 3.6465510528 4.1838691503 2.7914199269
C 3.3773471148 5.1494613005 3.2418289142
H 3.2367853944 3.4106648344 3.4519911094
H 4.7392968667 4.1119285573 2.8465084456
C 0.7642717477 3.1228403339 1.9319525773
H 0.123311551 3.9519891073 2.2627666956
H 0.0993733605 2.3864596018 1.4650597561
H 1.1692443587 2.6637847097 2.8414149756
C 2.1712814443 -1.8302853689 -0.3483512367
H 2.2521829059 -2.9175192134 -0.4868709884
H 1.6571915085 -1.6786525896 0.6081322043
H 1.501651322 -1.4680401823 -1.13746855
C 4.1197268596 -1.3911010592 2.1402919565
H 4.4561432083 -2.4208084964 2.3254404558
H 4.6395759223 -0.7609754192 2.8717587693
H 3.0524075063 -1.3654946317 2.3896382743
C 6.8310917851 -0.1133206154 1.0534189627
H 7.4935142211 -0.9888190263 1.1037282301
H 7.431088911 0.7038395329 0.6358966789
H 6.5946795613 0.1542956737 2.0900837046
C 6.5609985515 0.2346443059 -2.103946832
H 6.1569253623 0.693612428 -3.0138484807

H 7.2234254254 0.9720110069 -1.6351177361
H 7.2042945774 -0.5929523891 -2.434115163
C 3.6825105282 -0.8311382282 -2.9700428787
H 2.5896635516 -0.762354295 -3.0270721483
H 4.0912155144 -0.0558069546 -3.6287823164
H 3.9554001263 -1.7953030824 -3.4212910049
Sm 3.6591350886 1.6748482933 -0.0880826962

A_Sm (large core)

E: -964.832416092 ; H: -964.269328 ; G: -964.377556

Sm -0.129524 0.255398 -0.085487
H -3.063947 -2.829575 -0.557332
C -3.592003 -2.096806 0.062457
C -2.715544 -0.917821 0.344906
C -2.949034 0.356743 0.181285
C -2.927353 1.674046 0.094836
H -4.517314 -1.815955 -0.445040
H -3.845418 -2.599431 1.001470
H -1.812481 -1.163344 0.984935
H -3.285801 2.297263 0.911508
H -2.668724 2.175883 -0.837123
C -0.436884 -0.107777 2.912899
C -0.645265 -1.425206 2.374029
C 0.614499 -1.879721 1.848574
C 1.572295 -0.874524 2.082755
C 0.918340 0.226881 2.731077
C 0.334012 -0.320936 -2.832787
C 1.637838 -0.264478 -2.262538
C 1.902644 1.089362 -1.907232
C 0.763682 1.868696 -2.262020
C -0.202857 0.997767 -2.840380
C 3.205384 1.636502 -1.393439
C 0.666532 3.365669 -2.156108
C -1.504535 1.400951 -3.474461
C -0.314208 -1.532101 -3.443702
C 2.610593 -1.408310 -2.193869
C 0.862019 -3.251996 1.285443
C 3.047886 -0.941159 1.818193
C 1.618921 1.473492 3.191248
C -1.477389 0.685536 3.653856
H 3.066056 2.455812 -0.677172
H 3.806058 0.869042 -0.895021
H 3.824508 2.040462 -2.206869
H -0.372038 3.713299 -2.116543
H 1.172436 3.754675 -1.263847
H 1.129874 3.868954 -3.016338
H -1.828482 2.396601 -3.151364
H -1.426878 1.443766 -4.569859
H -2.320828 0.702785 -3.250437
H -0.079206 -1.627669 -4.513378
H 0.017464 -2.463121 -2.969733
H -1.407595 -1.498505 -3.368409
H 3.349538 -1.276426 -1.397117
H 2.111194 -2.367736 -2.016491
H 3.173077 -1.517789 -3.131740
H 1.823455 -3.315879 0.767104
H 0.870640 -4.021906 2.069960
H 0.087839 -3.552462 0.568136
H 3.316108 -1.792240 1.185535
H 3.433040 -0.037513 1.329989
H 3.612812 -1.049119 2.754468
H 0.915511 2.240640 3.529868
H 2.292890 1.267103 4.033772
H 2.243427 1.924890 2.408419
H -1.660623 0.281365 4.659589
H -1.185588 1.732853 3.782932
H -2.443694 0.675464 3.135330
C -1.589235 -2.395214 3.056050
H -2.577118 -1.966239 3.261263
H -1.739507 -3.319246 2.486611
H -1.161202 -2.686135 4.025916

TS_{A-I}_Sm (large core)

E: -964.791181530 ; H: -964.233175 ; G: -964.335419
Sm 0.3541070028 0.4697348491 0.2676801065
H -2.5846079602 -2.6261131414 -0.1986349163

C -3.0997628871 -1.8833776345 0.4210453369
C -2.2146498108 -0.6981671429 0.6806758931
C -2.4620466655 0.5616130134 0.5381989406
C -2.4279763205 1.8957068395 0.4533121463
H -4.034977156 -1.6136193021 -0.0816587675
H -3.3548497522 -2.3874898724 1.3600299114
H -1.0483288696 -0.9822583905 1.652811285
H -2.755904742 2.5228267871 1.2795815111
H -2.2524408478 2.3919260738 -0.4996949603
C 0.0577690327 0.1177875122 3.2808876846
C -0.1975910795 -1.2034397653 2.6842428934
C 1.115947824 -1.6689874809 2.203191067
C 2.0566099498 -0.6780828316 2.4424384177
C 1.3937415461 0.4407092044 3.0986606826
C 0.8204822571 -0.1069456572 -2.4782482376
C 2.1242968427 -0.0508562448 -1.9067941356
C 2.3892848823 1.3030512536 -1.5520395991
C 1.2503216214 2.0823528054 -1.9072463976
C 0.2844226714 1.211485699 -2.4865550128
C 3.6919540493 1.8504541424 -1.0386415409
C 1.1528272629 3.5793412817 -1.8013748663
C -1.0178907977 1.6145253282 -3.119331938
C 0.1721349502 -1.3181403905 -3.0888924486
C 3.0971691833 -1.194619555 -1.8392445527
C 1.3497771447 -3.036790313 1.6363677917
C 3.5322424573 -0.7289815242 2.1741877324
C 2.1039018204 1.6859174924 3.5469928641
C -0.9910286034 0.9031814902 4.0068299706
H 3.5530425335 2.6705653285 -0.3227121458
H 4.2947992749 1.0829394251 -0.5418059166
H 4.3119292658 2.2551909311 -1.8511844879
H 0.1141388239 3.9247527244 -1.7601848
H 1.6586364422 3.968747145 -0.9090435091
H 1.616312668 4.0823234467 -2.6618079754
H -1.3417582208 2.6087980419 -2.7941164103
H -0.9387790332 1.6562349513 -4.2146625562
H -1.8324597728 0.9165802313 -2.8914798754
H 0.4075948507 -1.4135186394 -4.1585360807
H 0.5032534282 -2.249335942 -2.6146680428
H -0.9204847599 -1.2838193386 -3.011061749
H 3.8383470344 -1.0631192993 -1.043785516
H 2.5978045978 -2.1545417476 -1.6627968923
H 3.6600774182 -1.3052989521 -2.7768309545
H 2.311456482 -3.1104531339 1.1211123915
H 1.346216817 -3.8012025293 2.425440578
H 0.5684866794 -3.3245800728 0.9227466016
H 3.8048214862 -1.5781259915 1.5423532921
H 3.9028330929 0.1790905851 1.6850283681
H 4.0947538372 -0.8287810672 3.1118210046
H 1.4039194691 2.4546536008 3.8857998296
H 2.7816929426 1.4755146568 4.3843697828
H 2.7232178065 2.1273742283 2.7558145012
H -1.1748847818 0.4862973447 5.0066527188
H -0.7053248861 1.9502169838 4.1431685992
H -1.947892392 0.8822847662 3.4740918417
C -1.0944934301 -2.1877515898 3.4300662084
H -2.0805913912 -1.7541687174 3.6245958572
H -1.2460901906 -3.1029865901 2.849525815
H -0.6546130983 -2.4713663058 4.3935456605

I_Sm (large core)

E: -964.804611992 ; H: -964.241301 ; G: -964.347840

Sm -0.260926 0.193012 -0.236885
H -3.435041 -2.588387 -1.176101
C -3.789496 -1.910545 -0.391543
C -2.832242 -0.781122 -0.169930
C -2.974114 0.471386 0.050133
C -2.707247 1.788915 0.236719
H -4.797859 -1.576528 -0.666299
H -3.882883 -2.520891 0.516157
H -1.396904 -1.476980 1.659170
H -2.794409 2.241556 1.223564
H -2.768859 2.477682 -0.604977
C -0.453339 -0.121471 3.026596
C -0.663554 -1.520467 2.492447
C 0.701663 -1.909865 1.966733

C 1.575970 -0.893695 2.209791
C 0.851713 0.228004 2.856012
C 0.302270 -0.340354 -2.966475
C 1.592762 -0.310260 -2.362911
C 1.862728 1.031708 -1.971243
C 0.740695 1.831222 -2.336504
C -0.219631 0.983507 -2.957680
C 3.153168 1.550172 -1.400267
C 0.653932 3.325600 -2.196059
C -1.514920 1.411777 -3.587563
C -0.345404 -1.530318 -3.617378
C 2.549722 -1.467289 -2.289819
C 0.968982 -3.255442 1.370680
C 3.052142 -0.863991 1.957972
C 1.531341 1.494582 3.280584
C -1.559339 0.645773 3.675462
H 2.998575 2.360220 -0.675692
H 3.726737 0.764537 -0.895629
H 3.811739 1.960359 -2.179325
H -0.382731 3.676839 -2.165103
H 1.144453 3.688546 -1.284067
H 1.138828 3.845590 -3.034489
H -1.842023 2.390353 -3.222016
H -1.426326 1.495652 -4.679811
H -2.329103 0.705730 -3.388344
H -0.083749 -1.608529 -4.682460
H -0.040118 -2.475325 -3.152726
H -1.438330 -1.480806 -3.563386
H 3.268112 -1.363213 -1.468781
H 2.033967 -2.425292 -2.152374
H 3.142869 -1.566124 -3.210165
H 1.944433 -3.302575 0.880015
H 0.950887 -4.039929 2.138921
H 0.207236 -3.528989 0.630857
H 3.389433 -1.740135 1.399882
H 3.356315 0.027116 1.398274
H 3.604851 -0.843515 2.905664
H 0.819087 2.230272 3.661454
H 2.260996 1.300045 4.076369
H 2.086548 1.960455 2.457751
H -1.794677 0.233479 4.665839
H -1.305851 1.699858 3.814328
H -2.477991 0.592236 3.081599
C -1.210740 -2.500883 3.543141
H -2.185238 -2.170472 3.914274
H -1.341691 -3.499453 3.116032
H -0.524168 -2.575772 4.392266

TS_{L-P}Sm (large core)

E: -964.788938055 ; H: -964.230716 ; G: -964.334437
Sm 0.3756521131 0.2773462275 0.1652004784
H -3.6154890275 -1.9245164046 -0.5913358427
C -3.3787888913 -0.9894854569 -1.1119753539
C -2.657650427 -0.0677724187 -0.2306752109
C -2.3567892733 0.8780437657 0.4998525028
C -1.7312373814 1.8062350764 1.37241907
H -2.7897713579 -1.254331661 -1.9966218722
H -4.3239754793 -0.5560365337 -1.4614709778
C 1.5177414315 0.5335134278 2.900593199
C 0.0733208689 0.3222774442 3.1168213005
C -0.1540854708 -1.1032380959 2.8172333712
C 1.0362087593 -1.6632249485 2.3797139747
C 2.079854614 -0.6493044814 2.4454175033
C 0.8611080456 0.1765788586 -2.6446163975
C 2.1419952382 -0.0498168719 -2.0633754349
C 2.5685228517 1.1637940935 -1.4536168504
C 1.5473090129 2.1379126134 -1.6532886781
C 0.4958178356 1.5301451605 -2.39570894
C 3.9266855843 1.4311130267 -0.8679752466
C 1.6310380439 3.5891970485 -1.2684364964
C -0.7264274347 2.2278405528 -2.922601683
C 0.0990806913 -0.804408379 -3.4915486349
C 2.9527017411 -1.3082717742 -2.2013716124
C -1.4634103922 -1.7955735177 3.0459924018
C 1.2819166486 -3.087333806 1.9708784056
C 3.5228152656 -0.9224882286 2.1379241849

C 2.2140910056 1.8236742296 3.2119241454
H 3.8951204957 2.1707094602 -0.0594747433
H 4.3904381624 0.5256907883 -0.4630697795
H 4.6200653574 1.8271763778 -1.6235883166
H 0.6405512874 4.0352345229 -1.1245537283
H 2.194631032 3.7424967183 -0.3405796508
H 2.1338907224 4.1895653991 -2.0398911488
H -1.0583702525 3.0373798731 -2.2631280638
H -0.5440679698 2.6798703349 -3.9078149493
H -1.5749025156 1.5455974988 -3.0388391582
H 0.4563342046 -0.8119571361 -4.5311527762
H 0.189994421 -1.8363820982 -3.1291647724
H -0.9690772749 -0.5652714384 -3.5335448235
H 3.6751629373 -1.4286818865 -1.3860579796
H 2.326225484 -2.2087013522 -2.2170922461
H 3.5336961528 -1.3213896036 -3.1345680813
H -1.5052277787 -2.7690548631 2.5488453511
H -1.6316568534 -1.9744816116 4.1170438749
H -2.3079096885 -1.2017554496 2.6814592854
H 0.347724249 -3.6331756322 1.8117291295
H 1.8710574114 -3.163413797 1.0486082135
H 1.8448611872 -3.6309413486 2.7408266936
H 4.1224605527 -0.0093306897 2.1478674831
H 3.9563156795 -1.6059740129 2.8794993788
H 3.6622888893 -1.3959744424 1.1589508165
H 2.2982745514 1.9781711482 4.2962422849
H 3.2275486543 1.8549408636 2.8026167463
H 1.6699506248 2.6911420655 2.8183012
C -0.5743380265 0.9271347092 4.3592408414
H -0.4263857558 2.0114805951 4.3943405163
H -1.653647254 0.7449837643 4.3675255879
H -0.1537915431 0.4979477089 5.2759748438
H -1.455677053 2.7542824247 0.8972552913
H -2.3030663857 2.0069637706 2.2816344078
H -0.631112321 1.0307643915 2.2355149654

P_Sm (large core)

E: -964.836885073 ; H: -964.273081 ; G: -964.382094
Sm -0.0544091946 0.0295617757 0.0742922847
H -3.4531516242 -2.0628556625 0.0018718648
C -3.6607718249 -1.2871202947 -0.741969493
C -3.3237605616 0.0394092907 -0.2341597558
C -3.1057066773 1.1590139344 0.1831801167
C -2.9118953098 2.520822991 0.6722421368
H -3.1025771457 -1.5235227662 -1.6541721404
H -4.7269802651 -1.3377398113 -0.9870641736
C 1.065920777 0.0436121977 2.7153865012
C -0.3096676972 -0.2596552473 2.9246371263
C -0.5557229812 -1.5655241752 2.4146071518
C 0.6665388632 -2.06977743 1.8866936822
C 1.6709393529 -1.0774719458 2.0782452708
C 0.2685945138 -0.1133773587 -2.7760499915
C 1.5721816007 -0.3337979737 -2.2464494629
C 2.0298207355 0.8914520307 -1.6831365423
C 1.0067248749 1.8669413011 -1.8628950988
C -0.0786921695 1.2479802722 -2.5457644722
C 3.4087728598 1.1615344994 -1.1502134243
C 1.1232116126 3.325723848 -1.5153792388
C -1.3065226163 1.9390244091 -3.0692377536
C -0.5344366899 -1.1039105399 -3.5731436105
C 2.3718570236 -1.5980129814 -2.3930418743
C -1.8456488762 -2.3252948852 2.5457316354
C 0.8991557923 -3.4570224514 1.3547103984
C 3.1401316413 -1.2607652685 1.8224164233
C 1.7807261809 1.2725552345 3.2057455248
H 3.4075195121 1.8985493935 -0.3384301741
H 3.8854516072 0.2557206078 -0.7636515184
H 4.0723400213 1.5599608645 -1.9309574449
H 0.1442265928 3.7991777473 -1.3751326102
H 1.6985905489 3.490885591 -0.5964579149
H 1.6313665955 3.8975276281 -2.3048204844
H -1.5297532418 2.858338949 -2.5163149038
H -1.1897696181 2.2326448824 -4.122030049
H -2.2014835078 1.3085974394 -3.0159116236
H -0.2209362304 -1.1333591039 -4.626517329
H -0.4356027523 -2.1303392813 -3.1972996715

H -1.6023738806 -0.8560317534 -3.5789079033
H 3.1199743513 -1.7082335964 -1.6008639977
H 1.7408039042 -2.4944892927 -2.3697529507
H 2.9180093331 -1.6273990175 -3.3466443943
H -1.942654727 -3.109468076 1.7851564613
H -1.9262169982 -2.8315015525 3.5182956136
H -2.7229511438 -1.6723164613 2.462826693
H -0.0057337054 -3.891440126 0.9134195672
H 1.6783945822 -3.4797348335 0.5844052043
H 1.2216301122 -4.1500860474 2.1447550739
H 3.6599860656 -0.3050703445 1.7033486434
H 3.6310459392 -1.7852877916 2.654581127

H 3.3383198353 -1.8520325732 0.9212736752
H 2.1349169422 1.1565876494 4.239841534
H 2.6622491034 1.5077665005 2.5990562304
H 1.1375596361 2.1611350375 3.1982762589
C -1.2938137444 0.5837503655 3.6859784645
H -1.0463344279 1.6513084893 3.6392909159
H -2.3197054378 0.4647254662 3.3167752481
H -1.3171085641 0.3225530781 4.7537184648
H -2.207083529 3.0765461701 0.0442030758
H -3.8612897728 3.0665826535 0.6587647413
H -2.5403165962 2.5267353455 1.7020628919

Eu

(Me₅C₅)₂Eu (large core)

E: -809.429556851 ; H: -808.960735 ; G: -809.048215

C 4.184274925 -0.6933767399 -1.5571883195
C 5.4707552195 -0.2187910602 -1.1702648255
C 3.509678998 -1.1420811609 -0.3849711738
C 5.591202943 -0.3739617779 -0.2408918609
C 4.3793719242 -0.9449493372 0.7263005578
C 1.8535962323 3.5733171768 0.995729299
C 3.1417816885 4.0456882081 1.3796890902
C 1.7307342341 3.7273370413 -0.4153466958
C 3.8150187382 4.4918512242 0.205722448
C 2.9427772787 4.2953857677 -0.9036654481
C 0.494830742 3.4530548065 -1.2276893277
H -0.1650115332 4.3305475084 -1.277084533
H 0.7282023287 3.1839478585 -2.2646065618
H -0.1065908531 2.6379466723 -0.8083287738
C 3.2066111482 4.7248519691 -2.3209637029
H 4.273106011 4.6962637018 -2.5732960692
H 2.6830072285 4.0966385421 -3.0513091679
H 2.872586048 5.7556419936 -2.5043877422
C 5.1609650733 5.1620494777 0.1634695079
H 5.8316048858 4.7998034267 0.9516554486
H 5.6732200766 5.0089388724 -0.793703087
H 5.0811857192 6.2494739207 0.3011216574
C 3.6527638166 4.1684825463 2.7891233597
H 3.382194187 5.1340388907 3.2387798399
H 3.2437615354 3.3951126344 3.4499046345
H 4.7455177009 4.0977931485 2.8446083869
C 0.7703815237 3.1076366918 1.9296798135
H 0.1306360596 3.9378235724 2.2602323747
H 0.1045724503 2.3719897779 1.4630582102
H 1.1748252937 2.6482593051 2.8391620402
C 2.1649365019 -1.8149051403 -0.3459471055
H 2.2470257979 -2.9019964279 -0.4848472088
H 1.6507147859 -1.6640066728 0.6105261014
H 1.4949673638 -1.4529614272 -1.1348489264
C 4.1136357975 -1.3761680585 2.1427108531
H 4.4500156643 -2.4061947591 2.3261241282
H 4.6339697613 -0.7470898808 2.8746545311
H 3.046520244 -1.3506299967 2.3927302644
C 6.8250614728 -0.0982122707 1.0558472528
H 7.4864724432 -0.9745111306 1.105458443
H 7.4256828335 0.7185148027 0.638509968
H 6.5892660463 0.1692809534 2.0926298168
C 6.5549028472 0.2498585038 -2.1016516546
H 6.1513609585 0.7091857093 -3.0115552929
H 7.2182489735 0.986471852 -1.6330674164
H 7.1969772491 -0.5787738874 -2.4315907886
C 3.6763020895 -0.8157065917 -2.96774908
H 2.5834538649 -0.7481381329 -3.02518356
H 4.0842734115 -0.0402263995 -3.6266984923
H 3.95052614 -1.7798421841 -3.4182399875
Eu 3.6591811294 1.67487148 -0.088082947

A_Eu (large core)

E: -965.355882140 ; H: -964.792711 ; G: -964.900429

Eu 0.0367509635 0.0075227072 0.1313785527
H -4.5194954387 -1.5824457227 -1.1804558478
C -4.7408670192 -0.8362395766 -0.4096154629
C -3.4842656568 -0.4374503387 0.3159196666
C -3.018548327 0.7855379845 0.3941830324

C -2.5519883736 2.0081417278 0.4816130047
H -5.2177925834 0.0228735154 -0.8850261349
H -5.4530579848 -1.2914495158 0.2875449049
H -2.9397176514 -1.2293120743 0.8354226476
H -2.8383391154 2.6642042859 1.3010993814
H -1.893822423 2.4224911691 -0.2821553927
C -0.2168487768 -0.5624661041 2.9372439152
C -0.1206971062 -1.8436219078 2.3221658125
C 1.1972721413 -1.984989513 1.8001763328
C 1.9173803045 -0.7919461792 2.0948296328
C 1.0409555637 0.0894499555 2.7906745665
C 0.2586506343 -0.4560002497 -2.6693108898
C 1.6013760535 -0.3244088905 -2.2132129468
C 1.8090287538 1.0359668044 -1.8459504827
C 0.5974018627 1.7464084389 -2.0854599869
C -0.3601235067 0.8253441736 -2.5991296737
C 3.1162632362 1.6562803058 -1.4379240207
C 0.4341106434 3.2374680208 -1.9723521062
C -1.7209106968 1.1627541394 -3.1423011039
C -0.3561256394 -1.6986471811 -3.2522100545
C 2.6533168334 -1.3963767294 -2.2680029598
C 1.765424303 -3.2378554605 1.1937376333
C 3.3827496494 -0.5640563088 1.8515970111
C 1.4150719626 1.4217275392 3.3793362371
C -1.3777749818 -0.0468039108 3.7415372822
H 2.9828170068 2.4910421145 -0.7392068169
H 3.7830205163 0.934602367 -0.9552572714
H 3.6615536283 2.0605234313 -2.3028160409
H -0.6190199705 3.5402567796 -1.9500961939
H 0.9123532325 3.649786728 -1.0746961588
H 0.8844057351 3.7616833609 -2.8270661542
H -2.1485280631 2.0597313559 -2.6808651058
H -1.687659883 1.3570614086 -4.2236807153
H -2.4426861303 0.3511474688 -2.9944321606
H -0.1872950306 -1.7721882966 -4.3360412177
H 0.0590208695 -2.6129133846 -2.8121531687
H -1.4426588123 -1.7318447739 -3.1069456698
H 3.4456136963 -1.2386122464 -1.5285889634
H 2.2401389189 -2.3957791433 -2.0916092843
H 3.1442032572 -1.4299642287 -3.2509574585
H 2.5608004269 -3.0269100209 0.4712945457
H 2.199966414 -3.89882824 1.9572853383
H 1.0019995125 -3.826828636 0.6719433604
H 3.748696543 -1.12838304 0.9873496376
H 3.6172486355 0.4910634467 1.6720487648
H 3.9899646969 -0.8787204413 2.7121654338
H 0.5681404923 2.1182099014 3.4070712429
H 1.7718785802 1.3285257662 4.4148947069
H 2.2195743603 1.9104441294 2.8179136289
H -1.2968265447 -0.3312101133 4.8002688611
H -1.4436267741 1.0469566518 3.7183865277
H -2.3401948146 -0.4328235084 3.3876057055
C -1.1573782728 -2.9328102219 2.3677981433
H -2.1551737691 -2.5418589446 2.5974818102
H -1.2319458797 -3.4934168146 1.4267031746
H -0.9334842022 -3.6744929602 3.1474279482

TS_{A-Eu} (large core)

E: -965.314867179 ; H: -964.756796 ; G: -964.858658

Eu 0.3527297198 0.4622660849 0.2697748133
H -2.5928820062 -2.6060392089 -0.2294712756

C -3.1006743518 -1.8683799878 0.4022064805
 C -2.2091333569 -0.6894926101 0.6678573715
 C -2.4475623655 0.5727531484 0.5322799557
 C -2.4020105758 1.9071589329 0.4570334004
 H -4.0386825544 -1.5898857887 -0.0904176507
 H -3.3503360461 -2.3818867461 1.3375472972
 H -1.04510433 -0.9816445267 1.6412558101
 H -2.7264891354 2.5307302027 1.2873500183
 H -2.2218268347 2.4087927538 -0.4921887248
 C 0.0576958546 0.119617804 3.2679066701
 C -0.1946991625 -1.2026043027 2.6716416434
 C 1.1197935843 -1.6653344919 2.1904388081
 C 2.0581210464 -0.6719371391 2.4287543654
 C 1.3926761038 0.4459116984 3.0844126061
 C 0.8159134354 -0.11611755 -2.460242575
 C 2.1196700456 -0.0577281998 -1.8888585272
 C 2.3825141224 1.2969203038 -1.534632911
 C 1.2422309053 2.0742469943 -1.8904338995
 C 0.2778598083 1.2015512759 -2.4696788131
 C 3.6853108698 1.8476016998 -1.024840359
 C 1.1435185671 3.5713286102 -1.7865822817
 C -1.0244716432 1.6020205246 -3.1041655347
 C 0.1689522418 -1.3288902217 -3.0692811842
 C 3.0945845796 -1.1998412919 -1.8228017055
 C 1.3570041152 -3.0328255864 1.6242514536
 C 3.5344128034 -0.7211919282 2.1641406413
 C 2.0999898054 1.6928735434 3.5324161436
 C -0.9923596559 0.9021999887 3.9950210573
 H 3.5468665834 2.6643354527 -0.30498154
 H 4.2933262195 1.0805133124 -0.5338476672
 H 4.2997617535 2.2577910133 -1.8388481841
 H 0.1046070614 3.9160922519 -1.7466362277
 H 1.6481144911 3.9621321488 -0.8942375976
 H 1.6074430096 4.0734237097 -2.6473077027
 H -1.3442583977 2.6006437547 -2.7885979352
 H -0.9467799934 1.6323466053 -4.1999455451
 H -1.8411908256 0.9093945724 -2.8678722784
 H 0.409931147 -1.4293363228 -4.1372446984
 H 0.4955842209 -2.2586853099 -2.5891600789
 H -0.9239174465 -1.2920170533 -2.9971550648
 H 3.837347901 -1.0665181547 -1.0292348521
 H 2.5973489085 -2.1604817691 -1.6443228521
 H 3.6552287656 -1.3101144629 -2.7617992523
 H 2.3196645169 -3.1045195308 1.110626158
 H 1.3535136189 -3.7970539868 2.4134904073
 H 0.5776926378 -3.3221685763 0.909102386
 H 3.8087998362 -1.5662130074 1.5276228553
 H 3.9062090115 0.1899602254 1.6820368534
 H 4.0938152296 -0.8271689555 3.1029843889
 H 1.3981069087 2.4603745908 3.870060192
 H 2.777386405 1.4842194811 4.3705553135
 H 2.7189510274 2.1350630108 2.7414636951
 H -1.1725179608 0.4856691441 4.9956639002
 H -0.7098824134 1.9503182738 4.1294978898
 H -1.9502243162 0.8774485407 3.464308417
 C -1.0900661449 -2.1888841613 3.4166473394
 H -2.0769018719 -1.7571000234 3.6113637121
 H -1.239991566 -3.1039206606 2.8353555531
 H -0.6498159066 -2.4724590982 4.3799523217

I_Eu (large core)

E: -965.328000718 ; H: -964.764687 ; G: -964.871310

Eu -0.316994 0.180211 -0.246901
 H -3.815576 -2.154638 -1.382792
 C -3.948017 -1.702352 -0.392813
 C -2.932734 -0.629875 -0.168664
 C -2.978568 0.624748 0.066187
 C -2.625274 1.918954 0.272453
 H -4.985169 -1.349338 -0.323230
 H -3.824913 -2.520108 0.328079
 H -1.425019 -1.573049 1.690469
 H -2.651390 2.349625 1.272396
 H -2.661522 2.630900 -0.550788
 C -0.465224 -0.169359 3.001122
 C -0.654209 -1.578527 2.490496
 C 0.701637 -1.947460 1.933359

C 1.559356 -0.909776 2.144355
 C 0.828121 0.204296 2.795034
 C 0.354795 -0.385555 -2.928585
 C 1.625896 -0.313900 -2.287418
 C 1.852168 1.041203 -1.913687
 C 0.722082 1.805979 -2.323749
 C -0.199112 0.925504 -2.958295
 C 3.119783 1.610008 -1.339263
 C 0.598667 3.300813 -2.220918
 C -1.483712 1.317676 -3.631341
 C -0.243210 -1.606404 -3.570608
 C 2.610915 -1.444321 -2.176364
 C 0.989712 -3.297527 1.357960
 C 3.029906 -0.856432 1.867610
 C 1.489970 1.491670 3.183099
 C -1.571289 0.583528 3.664676
 H 2.936030 2.373312 -0.571372
 H 3.749188 0.835919 -0.887506
 H 3.733770 2.096535 -2.110493
 H -0.446034 3.628400 -2.225783
 H 1.056796 3.695745 -1.305714
 H 1.093515 3.811071 -3.059746
 H -1.907722 2.233651 -3.206923
 H -1.339772 1.503835 -4.705081
 H -2.249715 0.539889 -3.542900
 H 0.058408 -1.707198 -4.623091
 H 0.065192 -2.532109 -3.070271
 H -1.338357 -1.581474 -3.558041
 H 3.309781 -1.307748 -1.343567
 H 2.118142 -2.413158 -2.030868
 H 3.223120 -1.543158 -3.084106
 H 1.960669 -3.332163 0.857913
 H 0.994645 -4.069554 2.138899
 H 0.227583 -3.598817 0.629154
 H 3.373367 -1.730585 1.310415
 H 3.309565 0.035851 1.297802
 H 3.595075 -0.820349 2.807438
 H 0.773626 2.211760 3.584790
 H 2.254792 1.322833 3.951091
 H 2.000962 1.964895 2.335856
 H -1.806888 0.152333 4.646747
 H -1.318030 1.634657 3.822351
 H -2.488909 0.540929 3.067755
 C -1.144616 -2.556476 3.571907
 H -1.217662 -2.246142 3.962757
 H -1.256817 -3.564992 3.163451
 H -0.434093 -2.597931 4.403613

TS_{L.P.} Eu (large core)

E: -965.312605186 ; H: -964.754340 ; G: -964.857426

Eu 0.3755963458 0.2870654132 0.1706898432
 H -3.6013174911 -1.9325142722 -0.5696078799
 C -3.3539905832 -1.0081722621 -1.1042052925
 C -2.6378322304 -0.075267195 -0.23061313
 C -2.3433667922 0.8782714639 0.4925018316
 C -1.7221641159 1.8144830665 1.3595397121
 H -2.7568710051 -1.2917602035 -1.9774690229
 H -4.2929904366 -0.5759693433 -1.4714204723
 C 1.5230546177 0.5327053907 2.8874979237
 C 0.0781040342 0.3281540865 3.1068210615
 C -0.1575357534 -1.095490987 2.8036045156
 C 1.0283859657 -1.6597529853 2.3598085759
 C 2.0776419271 -0.6514507619 2.4264318383
 C 0.8554625756 0.1735910334 -2.6252788023
 C 2.1365445567 -0.0495974266 -2.0429129699
 C 2.5612988813 1.1664754952 -1.4364743784
 C 1.5387186773 2.1386473466 -1.6390793792
 C 0.4882915222 1.5274809253 -2.3803278619
 C 3.9193319416 1.4389442664 -0.8528450489
 C 1.6212901974 3.5912386315 -1.2587241653
 C -0.7338793291 2.2227685359 -2.9106383132
 C 0.0965048433 -0.8103263453 -3.4716346892
 C 2.9495071201 -1.3067260602 -2.1803076321
 C -1.4688414134 -1.782465498 3.0369109975
 C 1.2654978486 -3.083711668 1.9453092679
 C 3.5187722097 -0.9323336932 2.1176838612

C 2.226966814 1.8184086226 3.200223463
H 3.8854531391 2.1731125484 -0.0394548444
H 4.3898775929 0.5339533848 -0.4551647598
H 4.6077662144 1.8443047236 -1.608050753
H 0.630271451 4.0386566493 -1.1234591651
H 2.1784117778 3.7475539254 -0.327429979
H 2.1301895737 4.1881729928 -2.0289047729
H -1.0720732967 3.0289779259 -2.2502373117
H -0.5481913287 2.6785591027 -3.8934948394
H -1.5792393776 1.5378774967 -3.0330556478
H 0.4592132289 -0.8229345305 -4.5093074942
H 0.1839436322 -1.8408288475 -3.1042351102
H -0.9709731598 -0.5697537913 -3.5201603469
H 3.6748238893 -1.4236945987 -1.3671291911
H 2.3249387628 -2.2085025089 -2.191601432
H 3.5273200122 -1.3207598304 -3.1154737439
H -1.5185996228 -2.7531701607 2.5351695799
H -1.6309267718 -1.965795777 4.1081670944
H -2.3125606518 -1.182749392 2.6805579265
H 0.3279219509 -3.6246435143 1.789511725
H 1.8491814109 -3.159644446 1.0195904344
H 1.8300855083 -3.632083841 2.7106589359
H 4.1227082857 -0.0220143809 2.1235782333
H 3.9497119289 -1.6152732582 2.8612915403
H 3.6542756759 -1.4099143331 1.1402867973
H 2.3148748405 1.9698669675 4.2846664071
H 3.2393649111 1.8452569338 2.7880251115
H 1.6864099777 2.689580899 2.8098957109
C -0.5643440615 0.9341007744 4.3513351641
H -0.4099832761 2.0174702867 4.3884538172
H -1.6446803228 0.7582203016 4.3607629572
H -0.1450071354 0.5005746493 5.266563127
H -1.447231528 2.7597413212 0.8786453972
H -2.2953395773 2.0196314683 2.2668983361
H -0.624178582 1.0403712832 2.2279252424

P_Eu (large core)

E: -965.360372509 ; H: -964.796448 ; G: -964.904907

Eu -0.042067 -0.042851 0.045052
H -2.754924 -2.706664 -0.177687
C -3.177770 -2.036226 -0.933292
C -3.186395 -0.651265 -0.471305
C -3.261233 0.497860 -0.084723
C -3.431971 1.873865 0.371892
H -2.605092 -2.148218 -1.859700
H -4.200347 -2.372625 -1.135093
C 1.179423 0.133741 2.607238
C -0.208747 0.000308 2.897211
C -0.607237 -1.322946 2.555227

Tm

(Me₃C)₂Tm (large core)

E: -812.495597829 ; H: -812.024736 ; G: -812.117250

Tm 0.8488822987 -0.1982699984 0.0664743559
C -0.2339116633 -0.1110727161 2.5868866241
C -0.2630748188 -1.4884581332 2.2202136597
C 1.0818356824 -1.9576878259 2.1620875516
C 1.942401602 -0.8701477535 2.4926546701
C 1.1292167822 0.271206414 2.755244246
C 0.5680147518 -0.6675223607 -2.6222943483
C 1.9311451976 -0.2851213065 -2.4541581663
C 1.960261221 1.0922322856 -2.0873673368
C 0.6153081564 1.5612844945 -2.0288931804
C -0.2452281281 0.4737062745 -2.3593922199
C 3.1961742326 1.9336107905 -1.9199498497
C 0.1871752122 2.9827417126 -1.7849450977
C -1.7385035989 0.5492834045 -2.5257831344
C 0.0807414912 -2.00375561 -3.1127509266
C 3.1303542912 -1.1474010839 -2.7400006636
C 1.5097408923 -3.379284677 1.9185758651
C 3.4356182448 -0.9457678155 2.6595396886
C 1.6166619058 1.6074659531 3.2454495532
C -1.433109492 0.7513224677 2.8724576646
H 3.0444939893 2.7637263331 -1.2203467723

C 0.532958 -2.005338 2.043361
C 1.639125 -1.107940 2.082268
C 0.202850 0.142413 -2.797963
C 1.499072 -0.234206 -2.344127
C 2.059951 0.875021 -1.648287
C 1.106635 1.933624 -1.665852
C -0.038479 1.482481 -2.382089
C 3.472505 0.978056 -1.146673
C 1.336477 3.325468 -1.144275
C -1.226435 2.318380 -2.768765
C -0.691526 -0.672691 -3.689601
C 2.206552 -1.520284 -2.672295
C -1.952473 -1.933461 2.834407
C 0.605395 -3.460015 1.667511
C 3.067411 -1.470630 1.787867
C 2.031608 1.327665 2.937086
H 3.557288 1.623305 -0.264951
H 3.886109 0.002182 -0.874192
H 4.140728 1.402551 -1.909558
H 0.405213 3.817206 -0.838111
H 2.006563 3.335614 -0.277289
H 1.795636 3.977072 -1.901232
H -1.354965 3.179161 -2.102149
H -1.122032 2.729993 -3.782727
H -2.164043 1.749256 -2.758446
H -0.472543 -0.505346 -4.754026
H -0.577219 -1.750958 -3.521696
H -1.750564 -0.425189 -3.550401
H 2.950464 -1.789585 -1.914446
H 1.514944 -2.366838 -2.760913
H 2.743596 -1.458355 -3.629420
H -2.112027 -2.850073 2.255681
H -2.058414 -2.215861 3.891328
H -2.784055 -1.257006 2.604039
H -0.350937 -3.844336 1.293070
H 1.355934 -3.649934 0.891405
H 0.878005 -4.092563 2.524229
H 3.672392 -0.592719 1.542179
H 3.546641 -1.953662 2.651335
H 3.158348 -2.171666 0.949792
H 2.424403 1.278160 3.962620
H 2.898856 1.413815 2.273584
H 1.474171 2.269120 2.864320
C -1.066069 1.025175 3.586639
H -0.831593 2.051716 3.276448
H -2.133068 0.857986 3.399392
H -0.937849 1.000098 4.678278
H -3.004571 2.585172 -0.341786
H -4.497145 2.106580 0.475867
H -2.963574 2.036560 1.348275

H 4.0493798636 1.351865889 -1.5522721648
H 3.5137805388 2.3832501977 -2.8710523938
H -0.8113034639 3.0455433839 -1.3370445872
H 0.8751427576 3.5167759292 -1.119215744
H 0.1464234327 3.5612747353 -2.7182931086
H -2.1930666349 1.2998849736 -1.8689530309
H -2.0200319996 0.8226293968 -3.5522033308
H -2.2304274383 -0.4070799958 -2.3137098555
H 0.0261308794 -2.039278221 -4.2096847661
H 0.7398571887 -2.8251566856 -2.808441056
H -0.9239262434 -2.2407304586 -2.7442196478
H 3.9993228351 -0.8686915593 -2.1326910152
H 2.9324028594 -2.2094233831 -2.5546701336
H 3.446961221 -1.06885033 -3.7893812562
H 2.5085828421 -3.4424227241 1.4715440005
H 1.5494856309 -3.957767771 2.8519989997
H 0.8221628808 -3.9131348071 1.2522903909
H 3.8902538089 -1.6970517752 2.0035472064
H 3.9277584891 0.0103271972 2.4467290682
H 3.7167992519 -1.2181835233 3.6863025698
H 0.9571060863 2.4287533371 2.9418111363
H 1.6722438296 1.6428848798 4.3423398866
H 2.6209631611 1.8447146948 2.8760722591
H -1.7502823662 0.6723704033 3.9216338485

H -1.2348112909 1.8133724606 2.6876898954
H -2.3018266633 0.4731047763 2.2645604893
C -1.4989310628 -2.329928575 2.0528456155
H -2.3526886182 -1.7477370987 1.6872052593
H -1.3479505325 -3.1588488661 1.3516527188
H -1.8152494934 -2.7812703302 3.0035725635

A_Tm (large core)

E: -968.421134593 ; H: -967.857750 ; G: -967.963837

Tm 0.1731182117 0.0388743928 0.1127885994
H -5.5085245051 -1.4739685996 -1.2482024915
C -5.2830797376 -1.0612030469 -0.2587197744
C -3.7962570161 -0.9121230935 -0.0783337118
C -3.1889818538 0.2202850893 0.1699773927
C -2.6076459581 1.3713836306 0.4228323501
H -5.7971478184 -0.1033877376 -0.1571225351
H -5.689687324 -1.7560079329 0.4844248758
H -3.1953374263 -1.818765925 -0.1569886995
H -2.4849725483 1.7236005707 1.4456921056
H -2.3020598219 2.0340972509 -0.3856584007
C -0.1644562773 -0.3634284003 2.8499473195
C -0.1231011999 -1.6702891145 2.2834526934
C 1.1951162669 -1.8964152645 1.7924073468
C 1.9684487926 -0.7284016021 2.0546601994
C 1.1262735393 0.2212961726 2.7028406323
C 0.3174170468 -0.396256485 -2.6157928748
C 1.6678306348 -0.3126104869 -2.1698690466
C 1.9174247338 1.0339514522 -1.7740668119
C 0.7221687105 1.7823692134 -1.982068954
C -0.2637031877 0.9003423964 -2.5105156159
C 3.2474208752 1.6040677295 -1.3665298242
C 0.5853192258 3.2705858588 -1.8081841969
C -1.6116579824 1.2909336751 -3.0500493205
C -0.3395755572 -1.5989918062 -3.2355527445
C 2.6891081899 -1.4124387797 -2.2535541752
C 1.7169513466 -3.1932715431 1.2379421761
C 3.4490156521 -0.5861500421 1.8400909339
C 1.5641793979 1.5491062141 3.2577664218
C -1.3124424839 0.2215014198 3.6239694534
H 3.1476700158 2.4303561262 -0.6527228198
H 3.8926498624 0.8525205237 -0.9011195686
H 3.7982298648 2.0032511618 -2.2300140886
H -0.450327625 3.5771696034 -1.619755784
H 1.189524823 3.6486100546 -0.9749774401
H 0.9126303969 3.8199026822 -2.7021557215
H -1.9275912231 2.2774658769 -2.693323453
H -1.6002850233 1.3519584615 -4.1472404892
H -2.4035883602 0.5793434283 -2.7864039246
H -0.1948001069 -1.6280935008 -4.3250237704
H 0.0617779415 -2.5408728949 -2.8442520453
H -1.4231585264 -1.6108591762 -3.0674585519
H 3.4800478269 -1.3012400201 -1.504338045
H 2.2457561774 -2.4042201789 -2.1107822442
H 3.1850950336 -1.4286518067 -3.2343323174
H 2.5281271284 -3.0413622325 0.5181354781
H 2.1159512832 -3.8421915712 2.0304191425
H 0.9366192119 -3.7696173705 0.7275765603
H 3.8031206342 -1.1837666272 0.9933613394
H 3.7447263163 0.4511864043 1.6502802944
H 4.0176650779 -0.9201182551 2.7196113329
H 0.7432827076 2.2748254748 3.2988068555
H 1.94893164 1.4572583322 4.2832812249
H 2.3664346579 2.0022686945 2.6641855947
H -1.2816467838 -0.076721153 4.6815204513
H -1.3030173363 1.3181455204 3.6159595307
H -2.2859288147 -0.1026637479 3.2381787675
C -1.225305006 -2.6915366034 2.3435720329
H -2.2190563895 -2.2299252809 2.3408320602
H -1.187934818 -3.394674138 1.5025545098
H -1.1664665126 -3.300881994 3.2566207653

TS_{A-I}_Tm (large core)

E: -968.379752004 ; H: -967.821551 ; G: -967.923248

Tm 0.3528904103 0.4032356055 0.273244017
H -2.6332830008 -2.4952474011 -0.3730735567
C -3.1038777292 -1.7761420366 0.3068517892

C -2.1720275435 -0.6376188767 0.6049476336
C -2.3588042126 0.6367840914 0.5067606827
C -2.2488265305 1.9692759326 0.4812051926
H -4.0456966838 -1.4480261425 -0.1463150917
H -3.3439029691 -2.3281272871 1.2226454702
H -1.0296812249 -0.974327355 1.5904378686
H -2.5498150051 2.5759311506 1.3325457979
H -2.0349704249 2.4958335884 -0.4467146298
C 0.0682812188 0.1327237691 3.2003024695
C -0.1863778179 -1.1964593017 2.618719437
C 1.1251893288 -1.6647565367 2.1358841547
C 2.0637382183 -0.6670304791 2.3555924252
C 1.4009466644 0.4595071609 3.0011053135
C 0.8051984568 -0.1640563541 -2.3764621516
C 2.1056914049 -0.0775931076 -1.8008896632
C 2.3353010132 1.2821867902 -1.4393727456
C 1.1773299699 2.0340265752 -1.796432568
C 0.23674747 1.1411092495 -2.384728666
C 3.6269013995 1.8667617266 -0.9380021974
C 1.0483454965 3.5290710277 -1.694206741
C -1.0674309141 1.5127814453 -3.0330949287
C 0.1899496589 -1.3886642684 -2.9949736489
C 3.1076198368 -1.196746282 -1.7488312198
C 1.3607249353 -3.0383631544 1.5841614716
C 3.5413452404 -0.7264512472 2.1031593991
C 2.1099801725 1.7115131868 3.4317156269
C -0.9755924562 0.917949051 3.9328687663
H 3.4750525598 2.6560578808 -0.1907647096
H 4.2722374384 1.10847926 -0.4830747447
H 4.2074759753 2.3226659747 -1.7524565172
H 0.0033128909 3.853708071 -1.6444629544
H 1.5524474151 3.9305451883 -0.80673783
H 1.4943980173 4.0378407412 -2.5604562241
H -1.3905888684 2.520787932 -2.7538979802
H -0.9860429423 1.5046359333 -4.1288242743
H -1.8825869808 0.8269279792 -2.7732524155
H 0.4526286666 -1.4859592986 -4.05814282
H 0.5220779594 -2.3126124136 -2.5072675173
H -0.9043307954 -1.3684985658 -2.9427624583
H 3.8698327863 -1.0356790268 -0.9799549571
H 2.6387108638 -2.1661338401 -1.5427233005
H 3.6413789667 -1.3059444214 -2.7034513346
H 2.3275410348 -3.1178165687 1.0798568882
H 1.3469817757 -3.7950442818 2.38045733
H 0.5871545974 -3.3308929458 0.8639965549
H 3.814328686 -1.5649624976 1.4578974188
H 3.925021879 0.1878617508 1.6383213576
H 4.0882087761 -0.8511091763 3.0471795746
H 1.4086500543 2.4837382355 3.7593924222
H 2.7875969738 1.5125802284 4.2720472799
H 2.7273692052 2.1422845828 2.6337425514
H -1.1427554384 0.5065067398 4.9378339472
H -0.693555242 1.9672525692 4.0571915083
H -1.9390254854 0.8875022865 3.4129116725
C -1.0869496547 -2.174414859 3.3673816718
H -2.0721887073 -1.7373657353 3.5583182462
H -1.2399223714 -3.091555111 2.7901955811
H -0.6494564184 -2.4552081324 4.3326893259

I_Tm (large core)

E: -968.392218061 ; H: -967.828607 ; G: -967.933704

Tm -0.219753 0.350679 -0.212031
H -4.388323 -0.910661 -0.058216
C -4.196159 0.072491 -0.504314
C -2.853548 0.597015 -0.115018
C -2.413260 1.703627 0.345110
C -1.582191 2.688453 0.777922
H -4.240752 -0.078456 -1.589514
H -5.025471 0.735567 -0.225909
C 0.713951 0.130223 2.814804
C -0.717643 -0.356617 2.876456
C -0.675222 -1.695806 2.174439
C 0.611897 -1.968766 1.824313
C 1.478404 -0.831039 2.226455
C 0.361070 -0.457153 -2.787284
C 1.640272 -0.423860 -2.157837

C 1.949057 0.935865 -1.861902
C 0.865971 1.741356 -2.316867
C -0.112903 0.880993 -2.893149
C 3.255603 1.452579 -1.326852
C 0.827701 3.244284 -2.324067
C -1.365606 1.322112 -3.595978
C -0.307290 -1.676288 -3.360908
C 2.585681 -1.586651 -2.047517
C -1.892685 -2.547207 2.016688
C 1.157175 -3.221878 1.211932
C 2.965423 -0.851036 2.053115
C 1.146605 1.425105 3.423111
H 3.128655 2.360470 -0.725254
H 3.768855 0.716372 -0.698419
H 3.953161 1.711518 -2.136267
H -0.198113 3.627254 -2.317197
H 1.342091 3.680194 -1.460034
H 1.312689 3.657445 -3.220024
H -1.825641 2.195157 -3.121013
H -1.165866 1.595172 -4.641895
H -2.123578 0.532488 -3.613503
H -0.019788 -1.847590 -4.408038
H -0.046440 -2.589977 -2.813809
H -1.399727 -1.593014 -3.345764
H 3.277244 -1.492005 -1.201897
H 2.060454 -2.542455 -1.937991
H 3.213207 -1.682098 -2.945386
H -1.700867 -3.428779 1.399871
H -2.257210 -2.900800 2.990141
H -2.709224 -1.981402 1.554901
H 0.362434 -3.898544 0.889544
H 1.793461 -3.011868 0.346313
H 1.778146 -3.764896 1.935502
H 3.424293 0.098546 2.336558
H 3.414733 -1.635555 2.674744
H 3.252460 -1.066105 1.018649
H 1.010199 1.415964 4.512406
H 2.200503 1.637704 3.227609
H 0.556773 2.264011 3.036481
C -1.235984 -0.470414 4.322071
H -1.236860 0.507186 4.812352
H -2.261186 -0.850647 4.335989
H -0.604985 -1.149839 4.903804
H -1.304601 3.502034 0.109586
H -1.501327 2.907542 1.842277
H -1.401473 0.331079 2.347278

TS_p_Tm (large core)

E: -968.377304274 ; H: -967.818853 ; G: -967.920723
Tm 0.3836250377 0.3209958703 0.1934786309
H -3.5001374279 -1.9754402614 -0.4732391284
C -3.2458909523 -1.0859469282 -1.0610682574
C -2.5456384492 -0.098937425 -0.2358188822
C -2.2619386819 0.8935869974 0.436881016
C -1.6441591671 1.8679978145 1.2640804661
H -2.6340357246 -1.4213431362 -1.9049754119
H -4.1795350185 -0.6795507952 -1.4689009821
C 1.5437693559 0.5283155811 2.8264717248
C 0.0953476511 0.3535111147 3.0477292881
C -0.1751348186 -1.0606525621 2.7250739307
C 0.9944542021 -1.6429001832 2.2611937789
C 2.0677473368 -0.6596762243 2.3400295902
C 0.8302804894 0.1542821152 -2.5263513614
C 2.1131028446 -0.0506574734 -1.9395016149
C 2.5244014233 1.1764771659 -1.3441723412
C 1.4915447693 2.1359318514 -1.5576351746
C 0.4492393608 1.5073642853 -2.2964762239
C 3.8790366149 1.4760261903 -0.7658816394
C 1.5623843051 3.5935123265 -1.1937938385
C -0.7735398474 2.1881968 -2.8435306725
C 0.092291297 -0.8429386159 -3.3757950789
C 2.9415426582 -1.2970489281 -2.0832144565
C -1.4951582852 -1.7254874456 2.9716169271
C 1.197418678 -3.0655986343 1.8245969962
C 3.5028760332 -0.9746460404 2.0387286956
C 2.2775626136 1.7934371113 3.1528481576

H 3.8302690942 2.1728445856 0.079276103
H 4.3872599434 0.5730838418 -0.413983072
H 4.539979894 1.9387295474 -1.5125076918
H 0.5678336876 4.0372692987 -1.0739993562
H 2.1086955414 3.7641823001 -0.2586564469
H 2.076435531 4.1825703011 -1.966669368
H -1.132638542 2.9886346167 -2.1872347392
H -0.5765677974 2.6477779454 -3.8223576416
H -1.6075241718 1.4925954829 -2.9798299431
H 0.4828024352 -0.8709738979 -4.4030512277
H 0.1685078701 -1.8678106321 -2.9906059506
H -0.9726894449 -0.6013459505 -3.4555784259
H 3.7034813077 -1.382040209 -1.3009553656
H 2.3345395933 -2.2101597194 -2.0465599223
H 3.4768797077 -1.3212454913 -3.0430982352
H -1.5796670628 -2.6790070615 2.4426214196
H -1.6315889796 -1.9372748936 4.0412421141
H -2.3334180223 -1.0968147773 2.6558666403
H 0.2469009504 -3.5863740767 1.6797333014
H 1.7620051509 -3.1403622866 0.8871708911
H 1.7654761811 -3.633110915 2.5732126529
H 4.1248153722 -0.0768251581 2.029246593
H 3.9164223715 -1.6517104975 2.7976212937
H 3.6293397655 -1.4736471062 1.071625919
H 2.3694098221 1.9308585533 4.2387923979
H 3.2895680878 1.8007830132 2.7391788407
H 1.7570714257 2.6805997473 2.7713984159
C -0.5364651321 0.9639081623 4.2949396283
H -0.3523584509 2.0420883235 4.3434385325
H -1.6212364357 0.8176761774 4.2974340602
H -0.1336751377 0.5100600874 5.2076612069
H -1.3549402591 2.7869104224 0.7427530385
H -2.2220567106 2.1184554874 2.1568319108
H -0.578727884 1.0877802086 2.1729762881

P_Tm (large core)

E: -968.424687861 ; H: -967.860621 ; G: -967.967490
Tm -0.0188521518 0.0157434835 0.078742643
H -3.3250725774 -2.0898712906 -0.0163422578
C -3.5120602366 -1.3095883252 -0.7603214186
C -3.1704293835 0.0117285354 -0.2416921923
C -2.9568168698 1.1313806965 0.1788610868
C -2.7838431273 2.4972978586 0.6650371545
H -2.9409859508 -1.547972305 -1.6636486164
H -4.5747603924 -1.3457919328 -1.0229138169
C 1.0485281442 0.0748923484 2.6359234776
C -0.3300936907 -0.2199688115 2.8393998804
C -0.5811936109 -1.5273902751 2.3325638734
C 0.6411301146 -2.0406833733 1.8124208715
C 1.6505440542 -1.0529037882 2.0062971275
C 0.2249727461 -0.1401683132 -2.6868844077
C 1.5365014949 -0.3509852772 -2.1708803609
C 1.9893196509 0.8766346238 -1.6085837173
C 0.9550520112 1.8443853926 -1.7743354947
C -0.1311437837 1.2188742339 -2.4513392073
C 3.3713897775 1.1647903353 -1.0936405218
C 1.075519322 3.3059060684 -1.4380623817
C -1.3567199995 1.906072914 -2.9851442322
C -0.5633913625 -1.1298340111 -3.5003608164
C 2.344246636 -1.6073353534 -2.3405795915
C -1.8689042852 -2.2860539484 2.4893670226
C 0.8721970603 -3.431932579 1.2894440673
C 3.1210097953 -1.2488332033 1.768180608
C 1.7708518031 1.2979593511 3.1307837994
H 3.3677302936 1.8609321362 -0.2464647282
H 3.8843171542 0.2569407695 -0.7635167237
H 4.001546796 1.6216348056 -1.8699631379
H 0.0978522633 3.7904260334 -1.3352918216
H 1.6231075266 3.4774970262 -0.5034513465
H 1.6144256315 3.8612401134 -2.2188213687
H -1.5825027955 2.8293200219 -2.4405004155
H -1.231380421 2.1905439911 -4.0393430996
H -2.252292808 1.277446337 -2.9301217879
H -0.2113145017 -1.1737317599 -4.5409431355
H -0.4943948608 -2.1540386433 -3.1117119371
H -1.6258757013 -0.8654934691 -3.547516176

H 3.129422309 -1.699990177 -1.5832854911
H 1.7269334523 -2.5114531463 -2.2786767959
H 2.8448401925 -1.6385858571 -3.3187746667
H -1.9577230494 -3.1042038574 1.7649654192
H -1.9495565758 -2.7474606521 3.4839119851
H -2.7487633727 -1.6417856834 2.3736001058
H -0.036001709 -3.8722228282 0.8618368742
H 1.6420637989 -3.4584550922 0.5100011729
H 1.2063180579 -4.1157742437 2.0825685507
H 3.6500023822 -0.2974741031 1.6577257733
H 3.5946831446 -1.7789146685 2.6067566309

H 3.3259348989 -1.8403275725 0.8689384728
H 2.1454089517 1.1652028669 4.1555867131
H 2.6393748369 1.5454381802 2.5103687999
H 1.1254929709 2.1841950634 3.1489282366
C -1.3070846732 0.6149697542 3.6189185255
H -1.0566016172 1.6821135886 3.5887619528
H -2.3352957697 0.5037560627 3.2544993546
H -1.3227814941 0.3343455314 4.6818524594
H -2.0038205734 3.0281496305 0.1086416984
H -3.7143670975 3.0611761441 0.5400184943
H -2.522802829 2.5123166431 1.7276298339

V.D Reactivity: (Me₅C₅)₂Eu(OEt₂) with HCCPh

1

E: -1043.03027542 ; H: -1042.412246 ; G: -1042.520435

Eu -2.4500343656 -1.4992134479 2.5747151402

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H -2.1154666737 1.7095543733 1.2797020067
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H -3.1532519948 3.4740251358 2.6698708401
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H -4.6882614109 3.2785961992 1.7979711534
C 4.1462877105 -3.205046756 -0.6092790153
H 4.3002334026 -3.3895925652 0.4578941102
H 3.4924655285 -3.992421336 -0.99192883
H 5.1129114112 -3.276888231 -1.1177453721
Eu -1.5115576635 -1.1693099983 0.5700602851
Eu 1.7690488933 1.1120589006 -0.6304385277

5

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O -1.3588962239 3.1137776939 1.8727148535
C 1.8347571504 -0.3195601601 0.1644017967
C 3.0382979025 -0.6232599886 0.2079774559
C 4.4280702602 -0.96361956 0.2673173101
C 5.3402686829 -0.4511713078 -0.6765283296
C 6.6900071615 -0.7832073487 -0.6147625773
C 7.1643661945 -1.6284645978 0.3884638441
C 6.2734973025 -2.1424390846 1.3313720551
C 4.9214839278 -1.818203934 1.2737444001
C 0.6001029409 -1.1944262979 3.9681918225
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C -1.5862455423 -0.4787713394 4.0531665592
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C -3.0869480386 -0.4924672152 3.9869235059
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C 2.99626994 2.8997814683 1.3334129285
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C 3.3646105868 3.8208223479 3.5280126977
C -1.1156202153 3.9609602466 0.7367251538
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V.E Reactivity: $(\text{Me}_5\text{C}_5)_2\text{Yb}(\text{OEt}_2)$ with $\text{C}_6\text{H}_5\text{PH}_2$

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C -3.260675597 -4.1534760839 3.2694002111
C -3.2587438672 -4.0361908643 1.8501966271
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H -4.365855179 -4.014272715 5.1336475318
H -5.3848787834 -4.0988676627 3.6997154162
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7
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TS₇₋₈

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C 5.6272137991 -1.5654773077 0.0756150141
H 4.4011705251 0.0015102829 -0.7295143284
C 5.6802748567 -2.7343456746 0.8349140058
H 4.5211906806 -4.1337820809 1.9960136766
H 6.5360347004 -1.163335496 -0.3666993347
H 6.6240795109 -3.2482529199 0.9937969999

V.F Reactivity: (Me₅C₅)U(NPh)₂ with H₂

TS_{direct}

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C 2.306394208 -0.8767361275 -0.9389068152
C 1.1574341116 -1.9013672986 -2.647817341
C 1.777920521 -2.0885201053 -0.4180143529
C 1.0700708538 -2.7596231143 -1.4771245532
C -0.6949673863 2.5050572144 -1.8861193328
C -1.7124780008 2.2712974571 -0.9100637254
C 0.406096723 3.1339826117 -1.232069219
C -1.2249675514 2.7224442643 0.3466677763
C 0.0880241735 3.2486819649 0.1487966452
C 1.6281546037 3.7207775738 -1.8802462418
H 1.5902189938 4.8169891807 -1.8423991962
H 2.5619535029 3.424747848 -1.3874642766
H 1.707156447 3.4427055665 -2.9340983356
C 0.9012879361 3.9755677501 1.1775901495
H 0.7634421844 3.5562543358 2.1770175606
H 1.971348006 3.9467710196 0.9494964267
H 0.6129516784 5.0350051368 1.2219221111
C -1.9959202509 2.8091124855 1.629678233
H -2.8459344088 2.1238001307 1.6396430544
H -1.3701409313 2.5756212326 2.4960272934
H -2.3890370941 3.8246752979 1.7731007952
C -3.1047302229 1.8111283489 -1.2170341234
H -3.7204509698 2.6588481797 -1.5470114157
H -3.1225186974 1.0642469145 -2.0155007108
H -3.5924210273 1.3646703951 -0.348406267
C -0.8524958462 2.2590169336 -3.3589137402
H -1.4996898376 3.0185629234 -3.8169730631
H 0.1038842852 2.2911264354 -3.8871784441
H -1.311394955 1.2863829903 -3.5669689468
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C 2.0459293905 -2.6941224539 0.925676767
H 2.7160243842 -3.5620557312 0.8504339062
H 2.5046402077 -1.9802238415 1.6141931182
H 1.1211365365 -3.0432099212 1.3997643913
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C 3.6682054725 -1.4140212301 -1.0343477538
C 5.1427331078 -0.1637838056 0.222204439
C 4.2235340635 -1.2540515844 0.2674375066
C 0.9854219578 3.1048907152 0.2090926154
C 2.0742879154 3.3688288418 1.0888480528
C 1.4557073533 3.2330449373 -1.1302401543
C 3.2281475492 3.6243710777 0.293111285

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C 0.6117279798 3.2066846525 -2.3680716408
H 0.2066931386 4.2054771929 -2.5815175978
H 1.1854638939 2.8998013237 -3.247880562
H -0.2331393281 2.5211424789 -2.2733625429
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H -0.9932648359 3.8159506139 0.6693563056
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C 3.9536638669 -1.0742058144 1.4975918326
C 5.4004577752 -0.1085692252 -0.0206554718
C 4.4359621735 -1.1440855251 0.1598587941
C 1.1166878199 3.217915434 0.274781052
C 1.9902233453 3.5061697122 -0.8156751527
C 1.8612878345 3.344223141 1.4815244306
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C 4.2371716272 4.1678500165 2.1079668943
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H 4.0246708528 5.2038482788 2.4053845435
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H 4.3889017099 4.0003653974 -2.1183448084
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H 1.2332253707 4.6679934708 -2.4545459463
H 0.7544948972 2.9704738863 -2.5026400705
H 2.3977305753 3.4284527676 -2.9380654817
C -0.3649410531 3.0058996403 0.1914212727
H -0.9018180517 3.9473941756 0.370486915
H -0.7136709858 2.2799560702 0.9303244563
H -0.6647033464 2.6384098208 -0.7929634161
C 3.1140872814 -2.1133323965 2.1733728739
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H 2.3718483408 -2.5485950317 1.4987590862
H 2.5712871168 -1.7111031276 3.0310510251
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H 0.9468367851 0.3221513848 3.9314926811
C -1.8951082913 -1.3748089099 3.1303978342
H -2.476325263 -1.9127181031 1.125215859
H -1.0466645117 -0.6966589286 4.9918663419
H -2.7696809123 -1.8218397863 3.5942536538
H 1.1507062946 0.8106011066 -0.9369540661
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2s

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C 2.6232686158 -0.3720632317 1.1422656408
C 1.235794544 -2.1920106389 0.9278060294
C 2.7205379401 -0.8424532483 -0.2025314677
C 1.8732105974 -1.9735677634 -0.3297762568
C -1.5559575358 2.3242940486 -0.2667130798
C -0.4403788828 2.5183165179 -1.1365711242
C -1.0800009445 2.4281093627 1.0773202877
C 0.7189357966 2.7209446819 -0.336359055
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H -1.3818924001 2.2166587859 3.2026140301
H -2.7928617856 1.8025537778 2.2346637235
C 1.1513331342 3.0404916037 2.2289648644
H 2.2156127017 3.077367194 1.9909187552
H 1.0199178628 2.3486874746 3.0678763148
H 0.8667915766 4.0360769818 2.5943408459
C 2.0613180457 3.1399494162 -0.8574892273
H 2.3048569686 2.6561108791 -1.8083154968
H 2.8676557391 2.9184611611 -0.1540709991
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H 0.4000245806 2.4070966992 -3.1310703411
C -2.9989985529 2.3840382573 -0.6775180925
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H -3.239159182 -1.9756835146 0.6432367722
C -3.205211007 -1.3846465898 4.4698389756
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C -4.229078561 -2.1424290345 3.900792722
H -5.0322935514 -2.9384537734 2.0649982722
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77
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C -1.0542265875 2.429203055 1.1563585913
C 0.7323423103 2.7896003489 -0.2565240263
C 0.3342742314 2.7197132139 1.1144193542
C -1.9139238148 2.4448332041 2.3839067486
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H,0,5.360541855,1.98872511,-3.6008355758
H,0,6.7692265026,2.1901522997,-2.5532209352
H,0,6.6832315244,0.8351618041,-3.681033871
C,0,3.9061449525,-0.6813794378,-3.6193341251
H,0,2.9533916929,-1.2145445011,-3.5966945181
H,0,3.7551466042,0.235153887,-4.1992537957
H,0,4.6201343003,-1.296300399,-4.1834061167
N,0,3.0546596556,0.8539748448,1.5879352933
N,0,1.0868219088,0.3091239169,-0.7095579179
H,0,4.1053217842,0.0485550943,0.8807232668
H,0,0.7569042725,-0.0610258672,0.1779378836
C,0,3.0762651919,0.5538632003,2.9346142655
C,0,1.9768581285,-0.0862302568,3.5478661705
C,0,4.1758587544,0.8862010778,3.7571715573

C,0,1.9812191685,-0.3771051404,4.907434009
H,0,1.1199450896,-0.345402518,2.9321637074
C,0,4.1750712418,0.5876435472,5.1160778683
H,0,5.0272069408,1.3907573844,3.3075065437
C,0,3.0795109409,-0.0460310079,5.7035395345
H,0,1.1186699838,-0.8689209104,5.3511264285
H,0,5.0367873813,0.8560397477,5.7229976256
H,0,3.0798600788,-0.2759089898,6.7651412678
C,0,0.252241622,-0.0706443379,-1.739199007
C,0,-0.8709652719,-0.9035102117,-1.5356813065
C,0,0.4964213587,0.3587651325,-3.0633650478
C,0,-1.6930547871,-1.2797848231,-2.5914641206
H,0,-1.0905859328,-1.2517576711,-0.5279638457
C,0,-0.3291699374,-0.0240054798,-4.1150140459
H,0,1.3479209677,1.0081079016,-3.2589268562
C,0,-1.433415567,-0.8477583609,-3.8932820178
H,0,-2.5493034079,-1.9206278086,-2.393626493
H,0,-0.1087302463,0.3295383162,-5.1197672197
H,0,-2.0786482952,-1.1432401053,-4.7150596943