

Suzuki-Miyaura Coupling Revisited: An Integrated Computational Study

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Supporting Information

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- A. Analysis of kinetic experiments to extract free energies
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- C. Optimized Cartesian Coordinates

A. Analysis of kinetic experiments to extract free energies

1. Estimate of rate constant for reaction of $\text{ArB}(\text{OH})_3^-$ with PhPdL_2X .

This section is based on ref. 30, B. P. Carrow and J. F. Hartwig, *J. Am. Chem. Soc.*, 2011, **133**, 2116-2119. The authors write: "In contrast, no reaction was observed between halide complex **3** and potassium p-tolyltrihydroxyborate (0.15 M) in the presence of PPh_3 (0.15 M) and 18-crown-6 at -30°C over the same period of time. In fact, less than 10% conversion of **3** occurred, even after 11 h."

From this we can estimate the rate constant. We take:

$$\frac{-d[\mathbf{3}]}{dt} = k[\mathbf{3}][\text{ArB}(\text{OH})_3^-]$$

Because of the low conversion, we can also write that the concentration of **3** is effectively constant, and hence:

$$0.1 = \frac{-\Delta[\mathbf{3}]}{[\mathbf{3}]} \times \frac{1}{\Delta t} = k[\text{ArB}(\text{OH})_3^-]$$

Using a time interval of 11 h = 4×10^4 s and $[\text{ArB}(\text{OH})_3^-] = 0.15$ M yields $k = 1.7 \times 10^{-5} \text{ M}^{-1} \text{ s}^{-1}$. At -30°C , this is equivalent to a free energy barrier of 19.6 kcal/mol. This value can be cross-checked using the T -dependent kinetics data provided in the SI, which also provide a more straightforward comparison to computation, since they report rate constants at room temperature, which is the temperature used in the calculations by Maseras et al. (ref. 32).

In the SI, kinetics are reported for $\text{ArB}(\text{OH})_3^-$ in excess, and $[\text{ArB}(\text{OH})_3^-]_0 = 0.15$ M. They report pseudo-first-order rate constants $k_{\text{app}} = k[\text{ArB}(\text{OH})_3^-]$, as a function of $1/T$, for T between 0 and 30°C (Figure S1, the curve for decay of reactant at one value of T is shown in Fig. S2). Fig S1 is an Arrhenius plot, the linear fit gives $\ln k_{\text{app}} = 29.3 - 1.05 \times 10^4 1/T$. For $T = -30^\circ\text{C}$ (243 K), this yields $k_{\text{app}} = 9 \times 10^{-7} \text{ s}^{-1} = k[\text{ArB}(\text{OH})_3^-]$, so $k \approx 6 \times 10^{-6} \text{ M}^{-1} \text{ s}^{-1}$, within a factor of three of our estimate above. However, for our present purposes, we can simply take the value

reported for $T = 25\text{ }^{\circ}\text{C}$, the same Arrhenius law yields $\ln k_{\text{app}} = -5.93$ or $k_{\text{app}} = 2.6 \times 10^{-3}\text{ s}^{-1}$ or $k = 0.018\text{ M}^{-1}\text{ s}^{-1}$. That gives $\Delta G^{\ddagger} = 16.1\text{ kcal/mol}$.

2. Estimate of the rate constant for $\text{PhPd}(\text{PCy}_3)_2\text{OH} + \text{Br}^- \rightarrow \text{PhPd}(\text{PCy}_3)_2\text{Br} + \text{OH}^-$.

Carrow and Hartwig write: "Equilibration was complete in the time required for acquisition of the ^{31}P NMR spectrum (<5 min).", starting from concentrations of $\approx 0.001\text{ M}$ of both reactants.

We assume that 5 minutes corresponds to at least 10 half-lives τ of the reaction, assuming constant concentration of Br^- . In practice, of course, $[\text{Br}^-]$ is not constant, but for the rough estimate of the activation free energy needed here, such a simple assumption is acceptable. Hence $\tau < 30\text{ s}$.

$$\tau \approx \frac{1}{k[\text{Br}^-]_{\text{so}}} k[\text{Br}^-] > \frac{1}{30\text{ s}}$$

This means that k should be larger than $30\text{ M}^{-1}\text{ s}^{-1}$ at 298 K . This translates to $\Delta G^{\ddagger} < 12.5\text{ kcal/mol}$ (assuming instead that the reaction time of 5 minutes must be only two half-lives gives a slightly larger upper bound for $\Delta G^{\ddagger}$ of 13.3 kcal/mol).

B. Tables

Table S1: Computed relative Gibbs energies for the monomeric route of transmetalation in 243.15 K in kcal/mol with $\text{P-}i\text{Pr}_3$ as the ligand.

3	0.0
5	-5.1
6	-8.1
10	8.7
12	10.7
TS1	21.2
14	3.4
16	7.0
TS3	16.3
18 + 19	-37.0

Table S2: Computed relative Gibbs energies for the dimeric route of transmetalation in 243.15 K in kcal/mol with $\text{P-}i\text{Pr}_3$ as the ligand.

8	0.0
20	9.7
TS4	14.7
9	-4.8
21	-5.9
10	1.8

Table S3: Computed relative Gibbs energies for molecules or TSs calculated with an explicit THF molecule at 243.15 K and 293.15 K in kcal mol. The reported energies are the difference in Gibbs energy $\Delta G(X \cdot \text{THF}) - [\Delta G(X) + \Delta G(\text{THF})]$. Species **15** returns a much lower Gibbs energy at 293.15 K in complex with THF; for this species, all energies in the main text refer to **15**·THF. Note that at the lower $T = 243.15$ K, many species are significantly stabilized by hydrogen-bonding with THF.

	243.15 K	293.15 K
3	4.6	6.1
4	0.0	1.4
5	2.3	3.9
6	2.6	4.3
8	2.4	4.0
9	-1.8	-0.1
10	0.0	1.6
11	-1.4	0.2
12	2.3	3.9
13	2.2	3.7
TS1	-2.1	-0.5
TS2	-2.4	-0.6
14	-2.5	-0.8
15*	-5.7	-4.0
21	-0.8	0.7
H ₂ O	0.6	1.4

C. Optimized Cartesian Coordinates

Below are listed the Cartesian coordinates for all species (in Å), as well as the B3LYP-D3BJ/DEF2QZVPP,DEF2TZVP(SMD)//B3LYP-D3BJ/SDD,6-31g(d)(SMD) single-point energies ("E"), and the calculated Gibbs energies based on the B3LYP-D3BJ single point energies and the thermal analysis using the B3LYP-D3BJ small basis frequency calculations (G293 and G243).

P(iPr)₃ COMPOUNDS

1:

E: -4427.815591

G293: -4427.212824

G243: -4427.197170

C	-0.00039700	4.47282600	-0.05847500
C	-0.00038300	3.81323900	1.16319900
C	-0.00025900	2.41340000	1.16940000
C	-0.00014600	1.67151800	-0.02250600
C	-0.00017500	2.38426400	-1.23236700
C	-0.00029600	3.78248800	-1.26298500
H	-0.00046800	4.38430900	2.08705400
H	-0.00025200	1.90605800	2.12692200
H	-0.00010200	1.84976800	-2.17740000
H	-0.00031400	4.32968200	-2.20099900
F	-0.00052000	5.83299100	-0.07591200
Pd	0.00000600	-0.34388000	-0.06554300
P	-2.38129700	-0.29959800	0.07186900
P	2.38131100	-0.29928900	0.07187400

C	-3.18855100	-1.58070800	-1.02350100
H	-2.79232800	-2.50700500	-0.59606000
C	-3.19370500	1.36967800	-0.22523600
H	-2.48783100	2.06654600	0.23474800
C	-2.93826000	-0.74475800	1.80304700
H	-4.01917300	-0.56972000	1.83127000
C	3.18876600	-1.58015100	-1.02363000
H	2.79214100	-2.50653800	-0.59675600
C	3.19349500	1.37010300	-0.22515500
H	2.48751300	2.06687100	0.23481600
C	2.93835700	-0.74450600	1.80301100
C	2.68389700	-2.21055700	2.16634800
H	3.00592800	-2.38389400	3.20129200
H	1.62388100	-2.46564600	2.08522700
H	3.24170700	-2.90052900	1.52622700
C	4.71925800	-1.62371300	-0.95740400
H	5.16908000	-0.75021000	-1.43950500
H	5.09250800	-1.67700200	0.07037300
H	5.08052100	-2.51458400	-1.48721400
C	2.68423300	-1.52315600	-2.47231100
H	3.08953400	-0.66725800	-3.01819600
H	2.99882600	-2.43268400	-2.99963600

H	1.59205200	-1.47835500	-2.50859600
C	4.55984200	1.58940700	0.43945500
H	4.91223400	2.59917600	0.19235700
H	4.51027200	1.52234700	1.52965800
H	5.31534100	0.88209900	0.08645800
C	3.26462400	1.70666500	-1.72110700
H	3.46891900	2.77718800	-1.84367000
H	4.07280600	1.15572900	-2.21211000
H	2.33154700	1.48498000	-2.24437900
C	-2.68331200	-1.52448200	-2.47196800
H	-2.99778500	-2.43422000	-2.99900000
H	-3.08822000	-0.66879600	-3.01846900
H	-1.59110500	-1.47986400	-2.50775200
C	-4.71908300	-1.62390700	-0.95797100
H	-5.08029300	-2.51492600	-1.48756500
H	-5.09283000	-1.67666900	0.06965200
H	-5.16848600	-0.75051400	-1.44066300
C	-4.56009300	1.58882000	0.43934400
H	-4.51053800	1.52176800	1.52954800
H	-4.91260200	2.59854500	0.19223600
H	-5.31549800	0.88141800	0.08633200
C	-3.26483700	1.70624800	-1.72118500
H	-4.07297400	1.15525900	-2.21220100
H	-3.46921700	2.77675700	-1.84373700
H	-2.33173700	1.48464600	-2.24445000
C	-2.68349400	-2.21072500	2.16651200
H	-1.62342300	-2.46559700	2.08541900
H	-3.00549300	-2.38404400	3.20147000
H	-3.24115300	-2.90087100	1.52644600
C	-2.26024500	0.18426200	2.81853600
H	-2.66070200	-0.00586500	3.82207400
H	-1.18052600	-0.00115100	2.84353500
H	-2.41406900	1.24324100	2.58973700
C	2.26014000	0.18428300	2.81858000
H	1.18045800	-0.00135500	2.84355000
H	2.66062300	-0.00585400	3.82210600
H	2.41374900	1.24331400	2.58988200
H	4.01923400	-0.56924800	1.83125200
Br	0.00017700	-2.97530500	-0.28825800

2:

E: -1211.189656

G293: -1210.867910

G243: -1210.856291

B	-0.22132900	-1.81970600	0.24806400
C	1.35067800	-1.51438100	-0.07105200
C	2.36133900	-1.87482900	0.83982800
C	1.76482700	-0.82270400	-1.22133400
C	3.70606800	-1.55180600	0.63751700
H	2.09348900	-2.43190100	1.73569500
C	3.10260800	-0.49028200	-1.46208600
H	1.01670300	-0.53465900	-1.95619500
C	4.04926200	-0.85659700	-0.51586300
H	4.47871900	-1.82992900	1.34838700
H	3.41164400	0.04200200	-2.35700500
F	5.35425400	-0.53044100	-0.72607000
O	-1.11541300	-1.35808000	-0.87242300
H	-1.01929000	-1.96671400	-1.61644600
O	-0.38055500	-3.22920800	0.54867600
H	-1.29203600	-3.33854900	0.86339300
O	-0.69772900	-0.92514200	1.37175500
H	-0.02711400	-0.92661300	2.06861100
Na	-1.34431400	0.68092300	-0.04337900
O	0.10528400	2.40261800	0.18306500
C	1.08433700	2.73516800	-0.83616300

C	0.74918800	2.38579100	1.47771300
C	2.43498300	2.86690200	-0.11890100
H	1.08832200	1.92327900	-1.57041400
H	0.77372300	3.66055000	-1.33236600
C	2.21259800	2.08506100	1.18428300
H	0.62228700	3.36557100	1.95808400
H	0.25227000	1.62454000	2.08589300
H	2.65021500	3.91847500	0.10010100
H	3.25599200	2.46512400	-0.71813600
H	2.87540700	2.40401000	1.99376000
H	2.34843900	1.01269800	1.01861400
O	-3.58647800	0.98077500	0.24376500
C	-4.33157800	1.06451900	-0.99874100
C	-4.06446300	-0.15648900	1.00339600
C	-5.23136900	-0.18032400	-1.05963400
H	-4.90031100	2.00037900	-1.00922500
H	-3.60703400	1.09107800	-1.82232100
C	-4.57257900	-1.13237600	-0.04899800
H	-3.22314800	-0.53316300	1.59056300
H	-4.86744500	0.17067900	1.67869000
H	-5.28680800	-0.59628300	-2.06948600
H	-6.24838600	0.06951700	-0.73818300
H	-3.71858300	-1.64981500	-0.49911900
H	-5.26750400	-1.87156300	0.36008300

3:

E: -1929.374913

G293: -1928.761188

G243: -1928.745544

C	-0.01784100	4.28764000	0.12848200
C	-0.02725700	3.56007400	1.31076400
C	-0.02423400	2.16194500	1.23515000
C	-0.01166800	1.47459300	0.00650200
C	-0.00290900	2.26592400	-1.15704900
C	-0.00605300	3.66455700	-1.11175300
H	-0.03681400	4.07899700	2.26522100
H	-0.03278900	1.60221000	2.16541800
H	0.00694000	1.78853300	-2.13338600
H	0.00078500	4.26369800	-2.01790700
F	-0.02037400	5.64892700	0.18715800
Pd	0.00592600	-0.55142700	-0.08644200
O	0.15600000	-2.63555200	-0.14131500
H	-0.69208500	-2.98924600	-0.44346900
P	-2.35213100	-0.60425600	0.01727200
P	2.35729600	-0.57072000	0.01332100
C	-3.07693000	-1.82694400	-1.20105700
H	-2.67734800	-2.78169000	-0.83719000
C	-3.23979200	1.04083100	-0.14073000
H	-2.56398900	1.71928900	0.38971000
C	-2.88392400	-1.25210900	1.68930200
H	-3.97203300	-1.14087900	1.75142000
C	3.02401600	-1.87903300	-1.13505700
H	2.53157500	-2.76632600	-0.72358000
C	3.24447100	1.05923100	-0.25469900
H	2.58799100	1.77317400	0.25405500
C	2.91742700	-1.11317200	1.71287200
C	2.55807700	-2.57719200	1.99608500
H	2.75885500	-2.80397500	3.05134000
H	1.50375400	-2.77375200	1.77896500
H	3.15608000	-3.26632900	1.39106100
C	4.54377600	-2.06983600	-1.09959500
H	5.06477500	-1.22306100	-1.55885800
H	4.92642700	-2.19139800	-0.08096300
H	4.81699500	-2.97007500	-1.66559300
C	2.50158900	-1.73102200	-2.57098100

H	2.98460000	-0.90918200	-3.10675500	C	1.89598700	-1.78010800	1.91499200
H	2.70610600	-2.65443300	-3.12825200	H	2.44383100	-2.72395400	2.01176700
H	1.42007500	-1.56509000	-2.57830000	C	-0.90721100	3.36789700	-0.96638600
C	4.64249300	1.17780900	0.36613500	H	0.05520900	3.47425900	-0.45513800
H	5.04617300	2.17545900	0.14980300	C	-3.47656500	1.78437600	-0.37340500
H	4.62679700	1.06276000	1.45356300	H	-3.70900200	0.81557100	0.08197100
H	5.34137100	0.44318000	-0.04515200	C	-1.71482100	2.72335500	1.79740000
C	3.27767200	1.44274800	-1.74023100	C	-0.35296600	3.28418800	2.22717900
H	3.53988300	2.50317100	-1.83953000	H	-0.38370400	3.53513000	3.29567300
H	4.03167200	0.86166900	-2.28095800	H	0.44852300	2.56181400	2.04737100
H	2.31216300	1.29140500	-2.22906300	H	-0.10149600	4.19908600	1.68079000
C	-2.52642700	-1.62702500	-2.62080000	C	-1.65316600	4.70561600	-0.95507300
H	-2.77426500	-2.49977700	-3.23785100	H	-2.59485900	4.64552000	-1.51117800
H	-2.95793400	-0.74638800	-3.10388000	H	-1.88010100	5.04892700	0.05963700
H	-1.43735900	-1.51153300	-2.61393200	H	-1.03706300	5.47710200	-1.43550100
C	-4.60575300	-1.93753700	-1.19003700	C	-0.57920400	2.90791300	-2.39361800
H	-4.91815500	-2.78697300	-1.81081000	H	-1.47193900	2.81720900	-3.01868000
H	-5.00256500	-2.09858700	-0.18242400	H	0.08431700	3.64227600	-2.86859700
H	-5.07449700	-1.03854200	-1.60143600	H	-0.06143800	1.94364300	-2.38338000
C	-4.61875100	1.13704300	0.52474400	C	-4.45122600	2.82161800	0.19941800
H	-4.57462000	0.95574300	1.60230200	H	-5.47068900	2.57095300	-0.12155900
H	-5.01150300	2.15197700	0.38144100	H	-4.44941800	2.83544000	1.29295400
H	-5.34102100	0.44011400	0.08998400	H	-4.23340200	3.83358000	-0.15515700
C	-3.30465900	1.51117300	-1.60047000	C	-3.67147600	1.63812100	-1.88857800
H	-4.06884700	0.96410600	-2.16155700	H	-4.67230600	1.23821300	-2.09276700
H	-3.56896100	2.57523400	-1.62846900	H	-3.59172100	2.60669300	-2.39258900
H	-2.34878500	1.39368900	-2.11606800	H	-2.94364500	0.95708800	-2.33643800
C	-2.53299200	-2.73425400	1.87348400	C	2.26172300	-1.21368900	-2.37433700
H	-1.48021800	-2.92415500	1.63737000	H	3.14259800	-0.87445500	-2.93253900
H	-2.71664400	-3.02642300	2.91518500	H	1.85913200	-2.08864600	-2.89151800
H	-3.14801000	-3.38161800	1.23935900	H	1.50979700	-0.41859200	-2.41485400
C	-2.23408300	-0.39918300	2.78746400	C	3.69213900	-2.66220300	-0.85170800
H	-2.60769500	-0.70844300	3.77158600	H	4.59351100	-2.37907600	-1.41065200
H	-1.14644600	-0.53096900	2.77815800	H	3.99479200	-2.88013200	0.17772400
H	-2.44407800	0.66867100	2.66777600	H	3.30873700	-3.58632100	-1.29546800
C	2.30150000	-0.18708900	2.77022000	C	1.13656300	-4.58796300	0.66948800
H	1.21389900	-0.31479400	2.80150800	H	1.16107300	-4.45876200	1.75514600
H	2.70230100	-0.43278800	3.76167000	H	0.59233300	-5.51910500	0.46492000
H	2.50864400	0.87023900	2.57561500	H	2.16373800	-4.72313200	0.31794200
H	4.00761800	-1.00758000	1.74391500	C	0.20100600	-3.75447900	-1.52292700
3-THF:				H	1.14159700	-4.01525000	-2.01855600
E: -2161.948290				H	-0.47180200	-4.61634700	-1.61048500
G293: -2161.221155				H	-0.25482200	-2.92201000	-2.06377800
G243: -2161.203533				C	2.86754800	-0.61885300	2.16198600
C	-4.12912600	-2.81394300	-0.28256600	H	2.42575200	0.33279700	1.84598400
C	-3.66424600	-2.43990600	0.97095600	H	3.11594900	-0.56767600	3.23024800
C	-2.55039500	-1.59448000	1.04564300	C	3.80439300	-0.75848900	1.61395200
C	-1.89157600	-1.11344100	-0.10228100	H	0.74970900	-1.76787900	2.93557300
C	-2.40903500	-1.52737500	-1.34384000	H	1.14940300	-1.88971300	3.95018700
C	-3.51974000	-2.37221800	-1.44883700	H	0.21075600	-0.81488700	2.89293600
H	-4.16388400	-2.80464900	1.86414500	H	0.02567600	-2.57083500	2.76054800
H	-2.19243000	-1.31014500	2.03099200	C	-2.19092100	1.64000100	2.77471400
H	-1.93867200	-1.18793100	-2.26320000	H	-1.45134300	0.83463300	2.84119700
H	-3.90852000	-2.68508900	-2.41379900	H	-2.31870600	2.06917600	3.77648200
F	-5.21193300	-3.63692300	-0.37033400	H	-3.14474800	1.19332600	2.47556700
Pd	-0.28477100	0.11776000	0.02379900	H	-2.44468700	3.54081400	1.79519200
O	1.29384800	1.47344100	0.21980000	C	4.34995200	2.46192900	-0.00310400
H	2.02699600	1.18394600	-0.34465800	O	4.04571900	1.58432300	-1.09737000
P	1.17635600	-1.72546300	0.18975600	C	5.28204600	0.96680700	-1.45435400
P	-1.66826200	2.01643600	0.06682900	C	5.96005300	0.63553400	-0.12000900
C	2.66098000	-1.53111000	-0.92609100	C	5.45856800	1.76402000	0.81715900
H	3.12268600	-0.62217400	-0.52792600	H	4.70607300	3.42561100	-0.39810600
C	0.42391200	-3.42900700	-0.03988400	H	3.41767100	2.61887800	0.54142400
H	-0.56315400	-3.31188200	0.41900800	H	5.05758100	0.09541500	-2.07409000
				H	5.89547700	1.66824100	-2.04330200
				H	5.62229500	-0.34213900	0.23836900
				H	7.05020800	0.60438800	-0.20654900

H	5.06442500	1.35462400	1.75116900
H	6.25684700	2.46737500	1.07213100

6-THF:

E: -2593.260854

G293: -2592.444929

G243: -2592.425254

Pd	-1.13689200	-0.03572100	0.11436100
P	-1.45369700	-2.36416100	-0.17324800
P	-0.81297200	2.24393500	0.69146200
C	-3.07409900	0.31181700	-0.32330500
C	-3.49929000	0.43854300	-1.65817700
C	-4.06349400	0.41600500	0.67126300
C	-4.84208600	0.64376100	-1.99566200
H	-2.77378900	0.37425300	-2.46380800
C	-5.41333800	0.61712800	0.36129300
H	-3.78678900	0.34041200	1.71896500
C	-5.77801200	0.72560600	-0.97365100
H	-5.16020300	0.74110400	-3.02973400
H	-6.17038800	0.69073400	1.13687700
O	0.85974600	-0.49367600	0.61788000
B	1.90239300	-0.38952400	-0.19065400
C	-0.87274600	-3.05676400	-1.81191800
C	-1.56520900	-2.31482600	-2.96261900
H	-2.65572500	-2.31094700	-2.86781200
H	-1.22710100	-1.27373200	-3.00200900
H	-1.31176100	-2.78961700	-3.91880600
C	-3.23645300	-2.94355300	-0.06874800
C	-3.55758300	-4.29980500	-0.71052000
H	-4.62721500	-4.50957300	-0.58035500
H	-3.35399300	-4.31194300	-1.78483600
H	-3.00255800	-5.12108500	-0.24782700
C	-0.41426500	-3.26019400	1.09524800
C	-0.52206100	-4.78826900	1.06559800
H	0.24866600	-5.22278900	1.71547100
H	-1.49412500	-5.12908000	1.43683800
H	-0.37762500	-5.20032700	0.06162300
C	-2.29166100	3.38647800	0.51926100
C	-2.29501300	4.63434000	1.41245800
H	-1.45223500	5.29874200	1.20034300
H	-3.21673000	5.20089100	1.22660100
H	-2.27558700	4.38769300	2.47763300
C	-0.41633100	2.33813100	2.51818800
C	0.94885400	1.72873500	2.85685000
H	1.01032800	0.69641100	2.50493100
H	1.77206600	2.28770400	2.39955900
H	1.09736600	1.75170400	3.94445900
C	0.67697300	2.98751100	-0.15284400
H	1.45078000	2.26782000	0.13084100
C	0.57994800	2.94613300	-1.68430100
H	1.58041600	3.07699200	-2.11312400
H	0.20252900	1.98330000	-2.03363500
H	-0.05680200	3.74648500	-2.07043900
C	1.09402400	4.37722300	0.34065700
H	2.07407100	4.63494200	-0.08169800
H	0.38572700	5.14555200	0.01443500
H	1.17819200	4.43188100	1.43047300
C	3.33345100	-0.90280700	0.29431900
C	4.23526700	-1.49828300	-0.60530500
C	3.73658500	-0.80606900	1.63743300
C	5.48335700	-1.97701400	-0.20072600

H	3.95485500	-1.59948400	-1.65039700
C	4.98700100	-1.25408100	2.06894400
H	3.05723600	-0.36630500	2.36222800
C	5.83730200	-1.83426300	1.13483000
H	6.17317600	-2.44587200	-0.89573200
H	5.30332800	-1.16747700	3.10402800
F	7.05218000	-2.28362100	1.54375000
O	1.80878900	0.12136100	-1.48612000
H	2.67529400	0.41730200	-1.83413000
H	-1.19088200	-4.10499700	-1.82510100
C	0.64858000	-3.01773000	-1.99236200
H	1.02160000	-1.99102500	-2.00823700
H	1.17928800	-3.56785600	-1.20943400
H	0.90463900	-3.48516600	-2.95242900
C	-3.75416500	-2.89470400	1.37526900
H	-3.38177000	-3.74439600	1.95638600
H	-3.46493200	-1.97505200	1.88961600
H	-4.84974300	-2.94610300	1.37357800
H	-3.76892900	-2.17182900	-0.63386500
H	0.59198200	-2.96360600	0.78451200
C	-0.59587900	-2.70544200	2.51503500
H	0.20709000	-3.09024800	3.15714400
H	-0.53395100	-1.61438600	2.51708900
H	-1.54772000	-3.00683100	2.96034400
C	-1.53226800	1.64755900	3.31531100
H	-1.34720500	1.75834000	4.39118100
H	-2.52065000	2.06715300	3.10079600
H	-1.56361800	0.57657400	3.08427000
H	-0.39993100	3.40019200	2.78586800
H	-3.11844200	2.74534500	0.84014700
C	-2.55926600	3.76989700	-0.94270400
H	-3.58102000	4.15789200	-1.03541400
H	-1.87571400	4.55664800	-1.27687700
H	-2.46480100	2.91795600	-1.62000300
F	-7.08867000	0.92073100	-1.28897300
C	4.39809700	2.26235600	-0.94028800
O	4.13606500	1.50563300	-2.13751100
C	5.38287900	1.06042900	-2.71524900
C	6.50269600	1.62549300	-1.83192700
C	5.79371100	1.84660800	-0.48754700
H	4.35539300	3.33595000	-1.17387000
H	3.61603100	2.02826800	-0.21516800
H	5.38505100	-0.03468800	-2.72202400
H	5.43646900	1.41592600	-3.75033700
H	7.35381000	0.94208100	-1.76165700
H	6.86214100	2.57994400	-2.23284800
H	5.74266000	0.91361600	0.08084900
H	6.27543400	2.60857700	0.13231600

5:

E: -2437.165004

G293: -2436.438362

G243: -2436.42015

Pd	-0.61587300	0.01848900	-0.00475500
P	0.62422800	-2.02669000	0.00155700
P	-1.87852100	2.02691900	0.25053900
C	-2.32594400	-1.02542900	-0.14806200
C	-2.84489900	-1.39913500	-1.39853300
C	-3.04861300	-1.41044600	0.99450000
C	-4.02669100	-2.13929400	-1.51380500

H	-2.32797200	-1.11503100	-2.30881200
C	-4.23091600	-2.15228200	0.90312600
H	-2.69504100	-1.13192400	1.98105100
C	-4.69788900	-2.50592300	-0.35555100
H	-4.42335100	-2.42523300	-2.48344300
H	-4.78256700	-2.45064300	1.78975500
C	1.27564500	-2.58278500	-1.65952100
C	0.13070000	-2.66452300	-2.67591800
H	-0.71813900	-3.25342400	-2.31430100
H	-0.23418800	-1.66092600	-2.91911500
H	0.49202500	-3.12535300	-3.60360100
C	-0.34876400	-3.50928800	0.61298400
C	0.19697500	-4.88764200	0.21757700
H	-0.45447100	-5.66206300	0.64268100
H	0.21015500	-5.03412300	-0.86603700
H	1.20752500	-5.06044300	0.59939400
C	2.16070300	-1.78100600	1.03377200
C	3.09549600	-2.99251800	1.12146400
H	4.04383000	-2.68274900	1.57908200
H	2.66930900	-3.78522500	1.74523200
H	3.32808000	-3.41723800	0.14029800
C	-3.73157500	1.90775400	-0.01593700
C	-4.58265100	3.00166000	0.64428900
H	-4.36258700	3.99473600	0.24286100
H	-5.64107900	2.79216900	0.44329300
H	-4.46048500	3.03776800	1.72992700
C	-1.73913900	2.64247200	2.01280700
C	-0.30851800	3.01195500	2.42612800
H	0.28547700	2.10932400	2.61439800
H	0.21565900	3.63054200	1.69285900
H	-0.33777600	3.56615700	3.37208500
C	-1.16540600	3.39823100	-0.79359500
H	-0.11791800	3.41743700	-0.47145200
C	-1.15553500	3.04531700	-2.29036200
H	-0.40031800	3.65388300	-2.80313600
H	-0.92811500	1.98747600	-2.46611400
H	-2.11736900	3.25257800	-2.76610500
C	-1.76020700	4.79204100	-0.56230400
H	-1.15789900	5.53435800	-1.10179500
H	-2.78526100	4.86412500	-0.93922600
H	-1.76158700	5.07665800	0.49464800
H	1.67847300	-3.58924600	-1.50242800
C	2.40092100	-1.68579900	-2.18267900
H	2.09286600	-0.63785800	-2.24870000
H	3.29306700	-1.73416700	-1.55289100
H	2.69053900	-2.02490800	-3.18651100
C	-0.58827900	-3.43582000	2.12715100
H	0.30680100	-3.73496400	2.68158200
H	-0.87380200	-2.43350000	2.45712300
H	-1.39736100	-4.12241000	2.40386300
H	-1.31705900	-3.38046500	0.11953300
H	2.66323700	-0.98894500	0.47129100
C	1.87407000	-1.20500300	2.42754200
H	2.80201500	-0.79223800	2.84135900
H	1.13577900	-0.39945100	2.38957100
H	1.51321600	-1.96924600	3.12101200
C	-2.30976000	1.60369800	2.98826300
H	-2.28087500	2.00057200	4.01054800
H	-3.34499000	1.33146900	2.76397100
H	-1.70795100	0.68812400	2.96559200
H	-2.35029300	3.55015000	2.06242600
H	-3.97863300	0.95493500	0.46232700
C	-4.08950200	1.78262800	-1.50386000
H	-5.11156300	1.39707700	-1.59913300
H	-4.05577700	2.75727000	-1.99997200
H	-3.42623700	1.09966100	-2.03884200
O	1.27692600	1.12642100	0.23414600

H	1.20830600	1.68092200	1.02253500
B	2.25954800	1.84703000	-0.70417300
O	2.07384500	3.25839300	-0.30042500
H	2.78891000	3.78813600	-0.68196900
O	1.91275500	1.56717000	-2.08496200
H	1.06298600	1.99277800	-2.26091100
C	3.76399400	1.30009700	-0.40108800
C	4.64031700	0.87653100	-1.41313800
C	4.24754800	1.22912200	0.91842200
C	5.92214500	0.38605900	-1.14001900
H	4.30296200	0.91650500	-2.44495500
C	5.51946700	0.74230100	1.22903700
H	3.60697600	1.55177900	1.73660800
C	6.33452000	0.32466700	0.18356000
H	6.59060400	0.05335700	-1.92894200
H	5.88084400	0.68381100	2.25163800
F	7.57622300	-0.15697600	0.46857400
F	-5.84618400	-3.22777900	-0.45630500

6:

E: -2360.682582

G293: -2359.982069

G243: -2359.964170

Pd	0.57460500	0.04505100	0.02836700
P	-0.19813000	-2.19582600	0.13283700
P	1.26939600	2.29574100	-0.18685200
C	2.48312800	-0.59024200	-0.01040800
C	3.18375100	-0.91886600	1.16362700
C	3.16938800	-0.74909900	-1.22838300
C	4.49954700	-1.39547800	1.13485600
H	2.70121400	-0.80767400	2.12981000
C	4.48302900	-1.22801000	-1.28480400
H	2.67692200	-0.49635400	-2.16336700
C	5.12488300	-1.54488100	-0.09532900
H	5.03360100	-1.64571200	2.04704700
H	5.00266100	-1.35346300	-2.23038500
O	-1.44615700	0.61377200	-0.08157200
B	-2.37950800	0.94624400	0.78668200
C	-0.72851500	-2.73630900	1.84414400
C	0.43128800	-2.54923000	2.83082400
H	1.35142400	-3.04069700	2.49983400
H	0.64787000	-1.48366000	2.96518400
H	0.15979800	-2.96542400	3.80903400
C	1.04994900	-3.50519700	-0.36810300
C	0.79558000	-4.92784100	0.14761200
H	1.60016100	-5.58365000	-0.20949700
H	0.79437900	-4.98281500	1.23979500
H	-0.15030200	-5.33896500	-0.21669900
C	-1.74784600	-2.36240600	-0.89871000
C	-2.36015800	-3.76622500	-0.93627000
H	-3.35046700	-3.71969500	-1.40757800
H	-1.74763400	-4.45641500	-1.52539600
H	-2.49031600	-4.19394800	0.06298300
C	3.11867900	2.61522600	-0.26319700
C	3.55721500	3.89338100	-0.99116800
H	3.16293000	4.79774500	-0.51832500
H	4.65266600	3.95777000	-0.96400600
H	3.25922700	3.89946500	-2.04318400
C	0.64682200	3.00503200	-1.80217400
C	-0.87320900	3.19930500	-1.82824400
H	-1.39096500	2.26346000	-1.60616100
H	-1.20196300	3.94838100	-1.10034400
H	-1.17521500	3.55145300	-2.82329000
C	0.49087100	3.35272200	1.13812600
H	-0.57458400	3.19203100	0.94498000

C	0.75572800	2.81059800	2.54983100
H	0.07796000	3.30181600	3.25817500
H	0.56385500	1.73573400	2.60146700
H	1.78004900	3.00420300	2.87861100
C	0.79688500	4.85105800	1.03789200
H	0.16396500	5.40362100	1.74442100
H	1.83934600	5.06502800	1.29483800
H	0.60405300	5.25181300	0.03739400
C	-3.91298900	0.77980000	0.37576900
C	-4.96971700	0.73026700	1.30178900
C	-4.24372200	0.61091700	-0.98187300
C	-6.29458700	0.52794100	0.90789900
H	-4.76970200	0.82978800	2.36734600
C	-5.55741700	0.41682100	-1.40794700
H	-3.44272300	0.62563300	-1.71436400
C	-6.56092800	0.37880900	-0.44669400
H	-7.10721800	0.48210900	1.62624100
H	-5.81037500	0.29186900	-2.45642900
F	-7.84386100	0.18458500	-0.84494300
O	-2.07616600	1.41946000	2.07450100
H	-2.87530100	1.67322200	2.55976700
H	-0.95888600	-3.80472500	1.76711000
C	-1.98079300	-2.01529100	2.35359900
H	-1.81139200	-0.94096900	2.46140300
H	-2.84621900	-2.16114300	1.70055000
H	-2.24447100	-2.41456600	3.34173800
C	1.26989100	-3.51283000	-1.88709400
H	0.44302300	-4.01110500	-2.40316400
H	1.37271500	-2.50487200	-2.29667300
H	2.18922900	-4.06334600	-2.12084300
H	1.97303700	-3.14177500	0.09479500
H	-2.42940100	-1.69234800	-0.36761900
C	-1.59114000	-1.77351300	-2.30731600
H	-2.58099800	-1.69015200	-2.77385200
H	-1.15335700	-0.77328700	-2.26303000
H	-0.97369200	-2.40246800	-2.95411300
C	1.10269900	2.09722300	-2.95380000
H	0.82008700	2.54114300	-3.91654600
H	2.18717300	1.94420200	-2.96114100
H	0.62510000	1.11338500	-2.87946500
H	1.12088300	3.98553400	-1.91850700
H	3.48221400	1.76060200	-0.84242900
C	3.77383500	2.53522800	1.12230900
H	4.86125900	2.45213200	1.00501400
H	3.57171600	3.43700200	1.70871100
H	3.43451000	1.66720100	1.69180300
F	6.40326000	-2.01222300	-0.13658300

10:

E: -1739.928995

G293: -1739.478428

G243: -1739.464696

Pd	0.21079700	-0.05494700	-1.01784300
P	1.12539800	-1.46553000	0.49573700
C	1.41086500	1.42872300	-0.45977800
C	2.77363700	1.52872600	-0.77487300
C	0.79710900	2.51591600	0.18826300
C	3.51114100	2.67478200	-0.45322900
H	3.28428400	0.71525600	-1.27867100
C	1.51915600	3.66544000	0.52067500
H	-0.25768200	2.47158200	0.44294300
C	2.86885100	3.71980900	0.19488900
H	4.56569600	2.75681600	-0.69901100
H	1.04933800	4.50514200	1.02397400
F	3.58007000	4.83142600	0.51912900

C	0.82853000	-0.94585600	2.26122200
H	1.00299900	-1.84498500	2.86265700
C	1.78900400	0.14195900	2.75478400
H	2.83425200	-0.17964400	2.71849200
H	1.69102400	1.06226900	2.17457000
H	1.55196400	0.37577300	3.80004500
C	-0.63703100	-0.51725100	2.42462700
H	-1.33719100	-1.28985200	2.09291400
H	-0.84478900	-0.30566800	3.48053200
H	-0.84658700	0.38869400	1.84722200
C	2.95814800	-1.75190900	0.34906800
H	3.36188400	-0.77229800	0.62930600
C	3.40334200	-2.03485100	-1.09344200
H	2.90816100	-1.37469800	-1.81290500
H	4.48589300	-1.88101700	-1.17653500
H	3.19198500	-3.06673800	-1.38458900
C	3.51165800	-2.79914700	1.32317400
H	3.21616700	-2.60449300	2.35873000
H	3.17794300	-3.80622800	1.05483300
H	4.60782400	-2.79095900	1.28190700
C	0.16284900	-3.06317700	0.31264600
H	-0.85636100	-2.69467700	0.15495300
C	0.56985300	-3.82984000	-0.95292500
H	1.52293800	-4.35001800	-0.81532200
H	-0.19150600	-4.58614400	-1.17759500
H	0.66103000	-3.17541600	-1.82534300
C	0.15494600	-3.98470800	1.53923100
H	-0.29337800	-3.50682700	2.41452000
H	-0.44742000	-4.87230100	1.30825200
H	1.15814700	-4.32706400	1.80923200
B	-2.22152500	0.00811000	-2.11809400
O	-1.12974100	1.07989700	-2.32543700
H	-0.84369700	1.03954200	-3.25409900
O	-1.44155400	-1.26957600	-1.83877700
H	-1.20103200	-1.68277900	-2.68572200
O	-2.97550300	-0.19217300	-3.32335200
H	-3.73687500	0.40466500	-3.33894300
C	-3.00159100	0.39159300	-0.75911600
C	-2.98548300	1.68688600	-0.21412900
C	-3.70367000	-0.59362200	-0.04193400
C	-3.62055200	1.99475900	0.99294000
H	-2.44742300	2.47138600	-0.73769800
C	-4.34863900	-0.31802200	1.16567200
H	-3.73318600	-1.60900000	-0.42881000
C	-4.28721300	0.97806500	1.66308200
H	-3.59955500	2.99562900	1.41376100
H	-4.88407700	-1.08331600	1.71962700
F	-4.90183100	1.25885300	2.84280300

10-THF:

E: -1972.510689

G293: -1971.945523

G243: -1971.929945

Pd	-0.31199400	0.23929400	-0.27470000
P	-0.51835300	-0.72729000	1.75925700
C	-1.16203700	-1.32667000	-1.16101900
C	-2.52985700	-1.63402400	-1.10429400
C	-0.34363700	-2.10176500	-2.00273600
C	-3.07191200	-2.68355000	-1.85588800
H	-3.19735100	-1.06001300	-0.46992500
C	-0.86627700	-3.15637500	-2.75633900
H	0.71875800	-1.88751200	-2.07261900
C	-2.22547500	-3.42958600	-2.66356500
H	-4.13040200	-2.92261700	-1.81463900
H	-0.23592400	-3.75942700	-3.40307700

F	-2.74130100	-4.45760200	-3.38764400
C	0.37059500	-2.36135100	1.91021900
H	0.48613600	-2.52478500	2.98747200
C	-0.40337900	-3.55570600	1.34101800
H	-1.36473500	-3.70485300	1.84185900
H	-0.58440300	-3.45012400	0.26946700
H	0.19114100	-4.46507100	1.49378500
C	1.76362600	-2.24285200	1.27563500
H	2.33720600	-1.40283400	1.67807700
H	2.33424300	-3.16076300	1.46263700
H	1.68765500	-2.10249200	0.19356500
C	-2.25518900	-1.05364300	2.34587000
H	-2.56782900	-1.87059600	1.68561800
C	-3.20226900	0.12605700	2.08843200
H	-3.08849700	0.52415000	1.07608200
H	-4.24017400	-0.20713800	2.21039700
H	-3.03174800	0.94372300	2.79326000
C	-2.34327400	-1.54478800	3.79565900
H	-1.68934900	-2.40143400	3.98599300
H	-2.08088900	-0.74987000	4.50050600
H	-3.37235800	-1.85610600	4.01361400
C	0.40571600	0.40052600	2.94053000
H	1.25406600	0.72308500	2.32718500
C	-0.40729400	1.65342400	3.28634700
H	-1.22088200	1.42403800	3.98188900
H	0.24860500	2.38624600	3.77120000
H	-0.83044100	2.12746800	2.39788400
C	0.95575700	-0.26540200	4.20899800
H	1.68021100	-1.05304900	3.98572700
H	1.47551600	0.49491400	4.80544400
H	0.16463400	-0.69081000	4.83335600
B	1.49219600	1.99173200	-1.12943200
O	0.49661400	1.24462900	-2.05902500
H	-0.12006000	1.90038400	-2.42388300
O	0.77303800	2.10317900	0.18781200
H	0.11038800	2.83207200	0.15046000
O	1.75315600	3.31680200	-1.63462100
H	2.43783000	3.27386500	-2.31750500
C	2.75197900	1.00262600	-0.91655900
C	3.07011300	-0.03382600	-1.81029400
C	3.56834700	1.13587100	0.22117700
C	4.13704600	-0.90987000	-1.58657700
H	2.45521400	-0.17247800	-2.69489600
C	4.64175400	0.27835400	0.47295000
H	3.34831100	1.92206900	0.93875300
C	4.90085200	-0.73635800	-0.44058200
H	4.37408600	-1.71463800	-2.27619300
H	5.26594200	0.38132000	1.35566900
F	5.93696800	-1.58521700	-0.20381700
C	-1.30555900	4.55270400	-1.34160500
O	-1.25111400	4.02119000	-0.00159600
C	-2.54850000	3.46964200	0.26212000
C	-2.93422400	2.76026500	-1.03495300
C	-2.30899500	3.66910900	-2.12069100
H	-1.65212000	5.59375300	-1.29517000
H	-0.28699600	4.52514000	-1.73192100
H	-2.46162500	2.81071400	1.12710900
H	-3.25184800	4.28163500	0.50114500
H	-2.47759700	1.76373200	-1.05269700
H	-4.01614400	2.64341200	-1.14590200
H	-1.81751100	3.08328400	-2.90487200
H	-3.06697400	4.28687300	-2.61089700

12:

E: -1739.924277

G293: -1739.475524

G243: -1739.461618

Pd	0.17297300	-0.60729700	-0.02034600
P	2.06979400	0.65154800	0.07620200
C	-0.93620700	1.04791100	0.01525900
C	-1.24853800	1.78140500	-1.13807600
C	-1.59789700	1.37929000	1.20906400
C	-2.21194800	2.79584200	-1.11737100
H	-0.75935100	1.55698300	-2.07994000
C	-2.56362900	2.38979900	1.25053900
H	-1.37139200	0.84369900	2.12562700
C	-2.85503100	3.07719700	0.08001200
H	-2.46711400	3.35413800	-2.01311300
H	-3.08342100	2.64054900	2.17028800
F	-3.79434300	4.05903100	0.10890300
C	2.28332200	1.65769400	1.63134600
H	3.35095800	1.89945700	1.67101100
C	1.50763500	2.97933400	1.64164100
H	1.81633000	3.64658100	0.83153000
H	0.43032800	2.82061700	1.56440400
H	1.70604200	3.49670000	2.58847800
C	1.93082600	0.78365500	2.84264200
H	2.50228600	-0.15063500	2.85862000
H	2.14703700	1.32714500	3.77024100
H	0.86675600	0.52422500	2.83753600
C	2.24139200	1.85230500	-1.33715900
H	1.43805100	2.56575500	-1.12140000
C	1.93682900	1.22142000	-2.70478400
H	1.07692100	0.54531100	-2.66412900
H	1.71384100	2.01515700	-3.42762500
H	2.79063400	0.65641500	-3.08654900
C	3.57638500	2.60737900	-1.35606900
H	3.80149800	3.08414100	-0.39708600
H	4.40486700	1.93932300	-1.61060500
H	3.53781100	3.39458700	-2.11908000
C	3.50245000	-0.55888700	0.10769700
H	3.11168900	-1.36328800	0.73932500
C	3.77582900	-1.15451800	-1.28088600
H	4.31634300	-0.44589200	-1.91584200
H	4.40107100	-2.04858700	-1.17380500
H	2.86151700	-1.44450800	-1.80798700
C	4.80100900	-0.03836700	0.73857100
H	4.67685400	0.21771800	1.79411000
H	5.55930200	-0.82939500	0.68284100
H	5.19660800	0.83670800	0.21468700
B	-0.20601400	-3.42089300	0.21334000
O	-0.26418300	-3.96209600	1.55094500
H	0.52217300	-4.51734400	1.66761200
O	1.07689400	-2.56374700	0.05625700
H	1.47764700	-2.80980300	-0.79324300
O	-0.06873100	-4.39112400	-0.86953300
H	-0.78821900	-5.03476000	-0.79543500
C	-1.49069400	-2.40115400	0.02145700
C	-1.85979600	-1.92819400	-1.26339000
C	-2.33088100	-2.02273000	1.09726800
C	-2.99595800	-1.13630000	-1.47288400
H	-1.26947800	-2.23326900	-2.12409400
C	-3.46489900	-1.23751900	0.91414000
H	-2.08017800	-2.37501400	2.09314100
C	-3.76849300	-0.80143900	-0.37310800
H	-3.26916900	-0.77349000	-2.45851800
H	-4.10222600	-0.94441000	1.74246200
F	-4.85362200	-0.00979600	-0.55047000

12-THF:

E: -1972.502414

G293: -1971.938987**G243: -1971.923214**

Pd	-0.10925200	-0.01658800	0.24596800
P	-0.13535600	2.25724300	0.18509300
C	-2.03168900	-0.06581000	-0.28110600
C	-2.44768200	0.01731800	-1.61865600
C	-2.99329200	-0.39621100	0.68862200
C	-3.77190000	-0.24265100	-1.98849200
H	-1.73730400	0.26916600	-2.39941300
C	-4.32168300	-0.65870400	0.33934200
H	-2.71274600	-0.45859700	1.73492200
C	-4.68483200	-0.57792500	-0.99814400
H	-4.09199500	-0.19155300	-3.02491900
H	-5.06370000	-0.92083300	1.08750600
F	-5.97399800	-0.83079500	-1.34795200
C	-1.32414900	3.07093800	1.36950700
H	-0.96991400	4.10298200	1.46349300
C	-2.77497400	3.12407200	0.87871800
H	-2.87678700	3.69254900	-0.05038300
H	-3.18937600	2.12684600	0.71980100
H	-3.38550500	3.62587800	1.63982100
C	-1.21360300	2.38681700	2.73888500
H	-0.18316500	2.36733300	3.10945000
H	-1.82686500	2.92232500	3.47375000
H	-1.56699600	1.35202800	2.68585900
C	-0.54635600	2.94790500	-1.49484200
H	-1.60155200	2.66954300	-1.59698700
C	0.21899400	2.25319300	-2.63154100
H	0.27039900	1.16920200	-2.48616500
H	-0.28918800	2.44845200	-3.58353500
H	1.24188500	2.62702100	-2.71795900
C	-0.43510000	4.47510300	-1.58832900
H	-1.00097400	4.98342500	-0.80145200
H	0.60714000	4.80275700	-1.52627700
H	-0.83207600	4.81091000	-2.55435300
C	1.55541200	2.83212500	0.75556400
H	1.80324300	2.09274000	1.52418400
C	2.60069800	2.69667300	-0.35827300
H	2.49049600	3.48991700	-1.10452400
H	3.60146100	2.79001600	0.07867400
H	2.54549100	1.73215200	-0.86652600
C	1.60506000	4.23106300	1.38426100
H	1.00634900	4.30131000	2.29648200
H	2.64371700	4.45491800	1.65836100
H	1.27160100	5.00945700	0.69102600
B	1.71142100	-1.67522100	1.57978700
O	1.45466800	-1.44213600	2.99118100
H	2.25878700	-1.03821800	3.35196200
O	1.93168000	-0.33487100	0.88169900
H	2.52636500	-0.45203400	0.10531200
O	2.92215400	-2.44725300	1.29152700
H	2.82907300	-3.31636100	1.70829100
C	0.34088600	-2.35022300	0.93764100
C	0.19835700	-2.55529100	-0.45844900
C	-0.72611900	-2.80733000	1.74922600
C	-0.93030400	-3.17660700	-1.01743800
H	1.00580900	-2.26970400	-1.12796800
C	-1.85194900	-3.42685400	1.22000600
H	-0.65171500	-2.66199300	2.82253100
C	-1.93472800	-3.59074000	-0.16273600
H	-1.03212800	-3.32117500	-2.08831800
H	-2.66968600	-3.76843000	1.84734800
F	-3.04582200	-4.16897700	-0.68138300
C	4.90652600	0.07967500	-0.81685000
O	3.67977700	-0.53129200	-1.28416500
C	3.93927100	-1.90094000	-1.67629200

C	5.29501100	-2.25282800	-1.07459700
C	6.02786100	-0.90705100	-1.14310200
H	5.02224400	1.04778100	-1.31316500
H	4.81934800	0.24679300	0.26362700
H	3.13436000	-2.52226000	-1.28286600
H	3.95007000	-1.95452800	-2.77369200
H	5.14952600	-2.55819700	-0.03409600
H	5.80255400	-3.05408400	-1.62007200
H	6.86257900	-0.82863500	-0.44028800
H	6.41186100	-0.73033000	-2.15479100

11:**E: -1663.429667****G293: -1663.004884****G243: -1662.991435**

Pd	-0.20038100	0.24492700	0.31623800
C	-1.68770900	1.55038200	0.07486900
C	-2.59103600	1.88307000	1.09861900
C	-1.74052900	2.29456400	-1.11719600
C	-3.51116700	2.92671900	0.94891100
H	-2.58906100	1.32430100	2.02977800
C	-2.65404700	3.34077400	-1.28622200
H	-1.06222200	2.06231000	-1.93486100
C	-3.52529400	3.63436700	-0.24567600
H	-4.20675700	3.18876100	1.74063600
H	-2.69561100	3.91700100	-2.20572900
F	-4.42065900	4.64531400	-0.40198000
P	-1.56008000	-1.51726100	0.01398000
C	-1.73482500	-2.45423800	1.61565400
C	-3.30890600	-1.20138200	-0.56253800
C	-0.65984100	-2.67195400	-1.14081600
O	1.67658400	-0.78756500	0.57453700
B	2.39429300	0.31526800	0.49657600
O	1.62600300	1.53598100	0.67551400
H	1.94846300	2.31862600	0.20037200
C	3.93732500	0.41765900	0.21876500
C	4.62714900	-0.71385700	-0.25389900
C	4.67822100	1.59597100	0.41980200
C	5.99419700	-0.68127400	-0.52408500
H	4.07493800	-1.63612800	-0.41095300
C	6.04801700	1.65591300	0.16087500
H	4.18712200	2.48856400	0.80064500
C	6.67770000	0.51041800	-0.30994600
H	6.52942300	-1.55121900	-0.89142400
H	6.62366300	2.56222900	0.31943000
F	8.00718900	0.55598200	-0.56823000
H	-2.42446300	-3.28177000	1.41311600
H	0.22909100	-2.91724200	-0.54926200
H	-3.60535000	-0.33265100	0.03381500
C	-0.16310300	-1.97561900	-2.41530300
H	0.38964600	-1.06145300	-2.17657000
H	0.51321100	-2.65126600	-2.95331500
H	-0.98248200	-1.71712900	-3.09106300
C	-1.41859100	-3.96636700	-1.45591500
H	-0.75191500	-4.65703600	-1.98690100
H	-1.77246100	-4.47458700	-0.55323700
H	-2.28039200	-3.77558800	-2.10296400
C	-2.34992900	-1.53992500	2.68349200
H	-1.65959100	-0.72638700	2.93345100
H	-3.29706700	-1.09516300	2.36167300
H	-2.54234600	-2.11567400	3.59662200
C	-0.39794900	-3.03465800	2.09316700
H	0.37431800	-2.26184800	2.15499900
H	-0.53238100	-3.47511600	3.08873500
H	-0.03288100	-3.82464400	1.42965600

C	-3.35139300	-0.78791000	-2.03916400
H	-3.16561700	-1.64272500	-2.69671400
H	-4.34805800	-0.39646200	-2.27500000
H	-2.62323600	-0.00608600	-2.26927800
C	-4.30475300	-2.33396900	-0.27647500
H	-4.39586800	-2.54918800	0.79166900
H	-5.29548500	-2.02695400	-0.63392900
H	-4.04005400	-3.26062300	-0.79296800

11-THF:

E: -1896.013733

G293: -1895.474218

G243: -1895.458935

Pd	0.51010000	-0.34101800	-0.47148700
C	1.66137900	1.29136100	-0.47853600
C	2.36082700	1.70258700	-1.62641300
C	1.64370100	2.16317800	0.62464600
C	3.01159400	2.94063300	-1.68193800
H	2.40413800	1.05649600	-2.49840300
C	2.28809100	3.40454400	0.58961400
H	1.11322100	1.88278000	1.53038400
C	2.96255900	3.76836100	-0.56817700
H	3.54851200	3.26074200	-2.57005100
H	2.26852800	4.07994200	1.43971500
F	3.59436600	4.97172300	-0.61220100
P	2.20315400	-1.65447700	0.20823600
C	2.75775600	-2.72463600	-1.21420000
C	3.76145200	-0.84136800	0.84498900
C	1.48889100	-2.83729100	1.46138600
O	-1.11714900	-1.78059800	-0.54874000
B	-2.01156600	-0.82757300	-0.76161000
O	-1.46114000	0.43293100	-1.19342000
H	-1.89083100	1.26134300	-0.85384100
C	-3.56745200	-0.96019300	-0.55622800
C	-4.08475300	-2.09817100	0.08863900
C	-4.48299900	0.01896100	-0.98238000
C	-5.45164100	-2.26148200	0.31089400
H	-3.39493600	-2.86835000	0.42233500
C	-5.85648700	-0.11925500	-0.77505600
H	-4.12214500	0.91329300	-1.48205300
C	-6.31183400	-1.26158800	-0.12839600
H	-5.85370800	-3.13711600	0.81092500
H	-6.56559000	0.63384400	-1.10400400
F	-7.64368900	-1.40625400	0.08234100
H	3.59504600	-3.32641000	-0.84249100
H	0.73119600	-3.35120600	0.85932700
H	3.88974300	0.00021500	0.15639600
C	0.73674900	-2.12702000	2.59550400
H	0.03200000	-1.38893300	2.19961800
H	0.16557200	-2.86891900	3.16717400
H	1.41438900	-1.62275400	3.28930300
C	2.48467100	-3.87367000	1.99403000
H	1.94605400	-4.62753200	2.58155000
H	3.01371200	-4.39522000	1.18998500
H	3.22884500	-3.41260000	2.65115400
C	3.24795800	-1.83928600	-2.36782900
H	2.41114400	-1.27818300	-2.79789300
H	4.01168600	-1.12037800	-2.05440900
H	3.67926000	-2.46631900	-3.15734400
C	1.64503600	-3.66772700	-1.68832100
H	0.73102700	-3.11501300	-1.92859600
H	1.97858500	-4.19493600	-2.59057800
H	1.39652900	-4.42390600	-0.93750700
C	3.56474600	-0.26768000	2.25408900
H	3.55713600	-1.06184700	3.00707800

H	4.39667100	0.40665200	2.48935500
H	2.63719800	0.30259700	2.34358100
C	5.02570400	-1.70920100	0.77839100
H	5.27253400	-2.00968100	-0.24335400
H	5.87252700	-1.12628300	1.16158100
H	4.94173400	-2.61108600	1.39130900
C	-1.62532700	3.78388400	-0.08286800
O	-2.50886500	2.63098100	-0.11020600
C	-2.92466300	2.29975900	1.23532600
C	-2.69600900	3.57077000	2.04494300
C	-1.42132500	4.12696100	1.39415300
H	-0.69487800	3.52489100	-0.59651600
H	-2.12130800	4.59414000	-0.62953300
H	-3.96605100	1.97294100	1.19068800
H	-2.30992600	1.46907900	1.60985100
H	-3.53424300	4.26353000	1.90777500
H	-2.58334500	3.36895800	3.11398000
H	-1.28388400	5.20025000	1.55225400
H	-0.54084500	3.60651500	1.78422300

13:

E: -1663.437665

G293: -1663.012386

G243: -1662.998988

Pd	0.11872800	0.64429900	0.20452500
C	-0.91403900	-1.05663000	0.04173200
C	-1.15143400	-1.90774400	1.13359200
C	-1.59474100	-1.32077600	-1.15901600
C	-2.05328800	-2.97362700	1.04577100
H	-0.63772800	-1.74063100	2.07582600
C	-2.50025000	-2.38211900	-1.26740500
H	-1.43266000	-0.68840000	-2.02774000
C	-2.71232600	-3.18847000	-0.15772700
H	-2.24697200	-3.62635500	1.89191500
H	-3.03247400	-2.58368100	-2.19232300
F	-3.58946800	-4.22334300	-0.25259000
P	2.11486800	-0.40981800	0.04575800
C	2.99315100	-0.33728900	1.68883100
C	2.10961500	-2.21769900	-0.42706400
C	3.15656700	0.60397000	-1.12138900
H	3.20552500	1.55638400	-0.58249800
O	0.95018900	2.62160600	0.32158200
B	-0.13512500	3.28610800	-0.07200300
O	-0.13065800	4.56715700	-0.60938700
H	0.79405800	4.86405500	-0.65809000
C	-1.55412800	2.54391000	0.00914400
C	-2.39452300	2.39723500	-1.12112800
C	-1.97086500	1.91533100	1.20984100
C	-3.57050800	1.65974300	-1.06807700
H	-2.11060400	2.87038900	-2.05726100
C	-3.16756300	1.18524700	1.28639700
H	-1.38424000	2.04470300	2.11625300
C	-3.93064200	1.06116400	0.14054200
H	-4.20918900	1.53532900	-1.93683300
H	-3.48616500	0.70990500	2.20800700
F	-5.07124900	0.33511000	0.18502200
H	3.92827200	-0.89502900	1.56379900
H	1.27526200	-2.61682900	0.15858900
C	2.45259200	0.89157500	-2.45464700
H	1.44184600	1.27860200	-2.29176700
H	3.02235500	1.65078100	-3.00473400
H	2.38515000	0.00316100	-3.08786800
C	4.57856100	0.06960500	-1.32820900
H	4.57715400	-0.85134600	-1.92006000
H	5.17008200	0.81412400	-1.87543000

H	5.09085600	-0.13133800	-0.38181700
C	3.33075500	1.10094800	2.09976400
H	2.44508600	1.74261200	2.07119600
H	3.73228400	1.09860900	3.12063600
H	4.08889100	1.54547100	1.44776700
C	2.13908800	-1.02937400	2.75929100
H	1.21101700	-0.47136300	2.92813600
H	1.87366500	-2.05569900	2.48607200
H	2.69148400	-1.06599900	3.70585100
C	1.77062400	-2.41069000	-1.91041000
H	1.55122600	-3.46880300	-2.09588800
H	0.89471600	-1.83031700	-2.21180500
H	2.61336700	-2.10293700	-2.54901700
C	3.37559200	-2.99642000	-0.04383600
H	3.55348300	-2.99848600	1.03505900
H	3.25345100	-4.04073600	-0.35700700
H	4.26870100	-2.60512200	-0.53889900

13-THF:

E: -1896.015235

G293: -1895.476122

G243: -1895.460782

Pd	-0.51428800	-0.37265900	0.19987000
C	-0.96324300	1.57176600	0.06160700
C	-1.37705700	2.33348200	1.16753400
C	-0.66445000	2.25647500	-1.12922500
C	-1.46664300	3.72838700	1.10414000
H	-1.62512000	1.84224200	2.10413300
C	-0.74778300	3.65067200	-1.21444500
H	-0.34662800	1.70396300	-2.00928400
C	-1.14705500	4.36046800	-0.09047200
H	-1.77487900	4.31873000	1.96214500
H	-0.50911200	4.18023000	-2.13212800
F	-1.23171400	5.71628400	-0.16201700
P	-2.67452900	-1.01963500	0.02726800
C	-3.27035800	-1.69331500	1.66029400
C	-3.93076600	0.27988500	-0.44796900
C	-2.70349900	-2.46517800	-1.14825500
H	-2.08174400	-3.18628000	-0.60678000
O	0.25567800	-2.35643500	0.32157200
B	1.52831900	-2.11106900	-0.00004500
O	2.41648000	-3.09332400	-0.38240500
H	3.32909400	-2.74548700	-0.48155700
C	1.99278000	-0.56160800	0.02093400
C	2.42936400	0.10561700	-1.15021500
C	1.89400000	0.21507100	1.20228000
C	2.74626700	1.45891700	-1.15219000
H	2.51403300	-0.45421100	-2.07797700
C	2.22788300	1.57887800	1.22407500
H	1.60095300	-0.26064900	2.13513100
C	2.63250500	2.17177200	0.04216400
H	3.06850700	1.97151000	-2.05300800
H	2.15330900	2.16868800	2.13149500
F	2.92635600	3.49247200	0.03512500
H	-4.32905400	-1.94116500	1.52269900
H	-3.61992800	1.14234900	0.15067200
C	-1.98205600	-2.17513900	-2.47147300
H	-0.98637900	-1.75728000	-2.29337300
H	-1.86133400	-3.11352000	-3.02675800
H	-2.54162700	-1.48247900	-3.10571900
C	-4.09401300	-3.06863800	-1.37596900
H	-4.72310000	-2.40654900	-1.97920800
H	-3.99355500	-4.01580700	-1.92043300
H	-4.61848600	-3.27938900	-0.43838800
C	-2.51819100	-2.96504900	2.07075900

H	-1.43501400	-2.81305700	2.04920400
H	-2.81602400	-3.24682600	3.08836800
H	-2.75135900	-3.80802000	1.41301000
C	-3.14905500	-0.60907400	2.73913100
H	-2.09542400	-0.37191600	2.92551200
H	-3.66169600	-0.31792600	2.46284300
H	-3.58807000	-0.96963000	3.67709400
C	-3.80511200	0.67048100	-1.92594600
H	-4.38270900	1.58437300	-2.10891700
H	-2.76900400	0.86782100	-2.21280900
H	-4.20474500	-0.11176200	-2.57887900
C	-5.38556600	-0.04995300	-0.08551300
H	-5.52596600	-0.19104500	0.98975700
H	-6.02215600	0.78990500	-0.39073100
H	-5.74940400	-0.94372100	-0.59990900
C	5.20973900	-1.71438300	1.04755900
O	5.02250400	-2.17616300	-0.30618700
C	5.68457200	-1.28192500	-1.22740500
C	6.45234100	-0.27170400	-0.36954400
C	5.63523100	-0.25434000	0.93037900
H	4.26909000	-1.86127900	1.58528700
H	5.98886000	-2.32268800	1.52796000
H	6.33405200	-1.87461700	-1.88058100
H	4.92268200	-0.79109300	-1.84277000
H	7.46984000	-0.62928700	-0.17483200
H	6.51942000	0.70874800	-0.84986000
H	6.21042800	0.08280900	1.79763400
H	4.75778800	0.38982700	0.82293900

TS1:

E: -1739.902227

G293: -1739.455365

G243: -1739.441428

Pd	0.05961800	-0.67664500	0.01270300
C	-1.48976400	3.84778400	0.14519000
C	-1.32018400	3.15479000	1.33676600
C	-0.84495200	1.84054900	1.28437800
C	-0.53835000	1.22197900	0.06188400
C	-0.73881600	1.95400400	-1.11739200
C	-1.21153900	3.27132300	-1.08616900
H	-1.55399700	3.63713800	2.28128200
H	-0.70932200	1.30102900	2.21725700
H	-0.52210400	1.50342100	-2.08243700
H	-1.36474200	3.84141400	-1.99770500
O	0.28240100	-2.86149300	0.06834500
B	-1.05896800	-2.98614000	0.63681000
H	0.25122600	-3.19166200	-0.84543300
O	-1.79862700	-3.99381600	-0.03141600
H	-2.75038700	-3.85268800	0.07223900
C	-4.60000500	-0.22129300	-0.47298000
C	-4.15208800	-0.25025100	0.84238000
C	-2.88907400	-0.78734300	1.09268300
C	-2.06820400	-1.30895500	0.07200100
C	-2.59366200	-1.26380900	-1.24082600
C	-3.84639900	-0.72308600	-1.52956900
H	-2.52586600	-0.80303500	2.11710300
H	-2.00766400	-1.66412100	-2.06586700
H	-4.24190100	-0.68403000	-2.54008800
O	-0.99015500	-2.92546400	2.04576200
H	-1.82985800	-3.21513600	2.43045100
H	-4.77938500	0.14768800	1.63440500
F	-5.82066300	0.30446700	-0.73598300
F	-1.94393800	5.12986000	0.18655200
P	2.28930500	-0.02200300	-0.16040700
C	2.63555400	1.70985200	-0.80360400

H	1.83532700	1.85521900	-1.53746300
C	3.19456900	-1.13250300	-1.36440700
H	4.16622600	-0.66459700	-1.55069400
C	3.14789700	-0.29976500	1.47356100
H	3.07189800	-1.38870400	1.58192100
C	2.41354600	-1.17797900	-2.68511300
H	2.97770700	-1.74221300	-3.43759500
H	1.44215200	-1.66811200	-2.54918200
H	2.22419700	-0.17663100	-3.08758600
C	3.45326800	-2.53950900	-0.81095800
H	2.53964200	-3.01305500	-0.44343600
H	3.86853600	-3.16916900	-1.60785900
H	4.17912900	-2.52650600	0.00774300
C	2.37530400	0.31177600	2.65029600
H	2.83549900	-0.01011100	3.59282500
H	2.38431700	1.40455200	2.63025900
H	1.33284100	-0.02240300	2.64976000
C	4.63270000	0.08161900	1.48898700
H	5.08854400	-0.25724500	2.42775600
H	5.18604900	-0.38035900	0.66504300
H	4.77004300	1.16527700	1.42626100
C	2.46779800	2.79075900	0.27372800
H	3.29669600	2.77283000	0.98809800
H	2.46794600	3.77577400	-0.20827300
H	1.53252400	2.68951300	0.82503000
C	3.97703900	1.88625600	-1.52989200
H	4.04955500	1.27326400	-2.43221700
H	4.07195500	2.93429300	-1.84039800
H	4.83066300	1.65484100	-0.88578200

TS1-THF:

E: -1972.487865

G293: -1971.925779

G243: -1971.910076

Pd	0.13576700	-0.07049000	0.34486300
P	0.50111900	-2.31907400	0.00278500
C	2.05163500	0.34346600	-0.04550400
C	2.54263600	0.46767600	-1.35363500
C	2.93073900	0.62936500	1.01336200
C	3.86593200	0.85002100	-1.60622100
H	1.89542400	0.26889900	-2.20205200
C	4.25567900	1.01173000	0.78364400
H	2.58883000	0.55373200	2.04171000
C	4.69983800	1.11106400	-0.52876900
H	4.24439400	0.94653200	-2.61959700
H	4.93417200	1.23012500	1.60299200
F	5.98880500	1.47783100	-0.76323900
C	1.78154600	-3.13276400	1.08990400
H	1.58111600	-4.20794600	1.03166100
C	3.22717100	-2.90445800	0.63245000
H	3.41908900	-3.33291700	-0.35564300
H	3.48459300	-1.84380200	0.60397500
H	3.90518400	-3.39661000	1.34110800
C	1.57077800	-2.67289800	2.53896300
H	0.54355200	-2.84037400	2.88109900
H	2.24212200	-3.22365200	3.20902000
H	1.78990900	-1.60474600	2.64070000
C	1.02628000	-2.70564100	-1.74281700
H	2.03723200	-2.28173600	-1.76619000
C	0.19834400	-1.95017200	-2.79364200
H	0.02077400	-0.91035900	-2.49976700
H	0.73596000	-1.94915200	-3.74964200
H	-0.77351400	-2.42125800	-2.95984200
C	1.11806600	-4.20246300	-2.06195400

H	1.72981900	-4.74566000	-1.33484200
H	0.12606900	-4.66405000	-2.08610800
H	1.57317500	-4.34111500	-3.05068400
C	-1.09810000	-3.20259900	0.43285900
H	-1.45014000	-2.63358300	1.30095000
C	-2.14779200	-3.03712000	-0.67361300
H	-1.92288300	-3.67864400	-1.53152800
H	-3.12850400	-3.33553200	-0.28576200
H	-2.22627400	-2.00619900	-1.02597400
C	-0.96550700	-4.67532700	0.84090300
H	-0.35657700	-4.80663400	1.73961300
H	-1.96414700	-5.07254400	1.06275200
H	-0.53631600	-5.28768100	0.04188600
B	-1.72797200	1.17269200	1.67821700
O	-1.16352500	1.04206300	2.97764000
H	-0.42221100	0.41769400	2.94908500
O	-1.94203600	-0.09625000	0.98408700
H	-2.57154400	0.02031600	0.22686800
O	-2.85486500	2.02402700	1.59025300
H	-2.67304600	2.84131800	2.07711800
C	-0.35261400	2.09581000	0.56957000
C	-0.66900100	2.49293000	-0.75032400
C	0.51026600	2.94746300	1.28917600
C	-0.16108300	3.65775800	-1.32794600
H	-1.33209700	1.87536700	-1.35196300
C	1.02183500	4.12782900	0.75113300
H	0.77847200	2.68326700	2.30873800
C	0.68049300	4.45221700	-0.55762400
H	-0.40183300	3.95315800	-2.34483200
H	1.67913700	4.78373900	1.31417100
F	1.18049900	5.58948800	-1.09950900
C	-4.86717900	-0.75238900	-0.55170600
O	-3.78303700	0.10051300	-1.00457000
C	-4.28444100	1.44279500	-1.22339500
C	-5.57547800	1.52436400	-0.42004900
C	-6.13514300	0.10506600	-0.58518700
H	-4.91910400	-1.62661800	-1.20740100
H	-4.62974100	-1.08829200	0.46422400
H	-3.52156400	2.14278200	-0.88327500
H	-4.46234500	1.58005700	-2.29875900
H	-5.33229500	1.72719400	0.62775800
H	-6.25112800	2.30228300	-0.78779200
H	-6.84138700	-0.17810800	0.20052000
H	-6.64002200	0.00491900	-1.55288500

TS2:

E: -1663.394805

G293: -1662.974473

G243: -1662.960798

Pd	0.19791400	-0.52128300	-0.05819400
C	0.36151000	4.26154200	0.16287900
C	0.46600400	3.63721400	-1.07279900
C	0.44058700	2.23949300	-1.12245100
C	0.29740500	1.46759500	0.04218600
C	0.21362300	2.14084900	1.27145600
C	0.24133400	3.53864000	1.34155700
H	0.57076100	4.23437400	-1.97376700
H	0.53398500	1.75432500	-2.08973400
H	0.11342900	1.58084500	2.19596600
H	0.17078600	4.05997000	2.29167200
O	0.31232300	-2.86420500	-0.06633500
B	1.32913000	-2.71468000	0.63870600
O	2.30797800	-2.95469900	1.49622700
H	2.92660600	-2.20004500	1.56827400
C	5.07190000	-0.52322900	-0.37490500

C	4.49395200	0.00681100	0.77411200
C	3.09882600	0.02782800	0.86922400
C	2.26955200	-0.49165700	-0.14894500
C	2.91444700	-1.01831500	-1.28735500
C	4.30857200	-1.03261100	-1.41511800
H	5.12700200	0.40252100	1.56275500
H	2.64940100	0.46728100	1.75656900
H	2.32182000	-1.43692600	-2.09773000
F	0.38331400	5.62082500	0.22051600
F	6.42432300	-0.54435400	-0.47736000
H	4.79734200	-1.43892900	-2.29552300
P	-2.18220900	-0.55337400	0.00276300
C	-3.01288400	1.08854400	-0.34429300
H	-2.37787400	1.79098900	0.20769900
C	-2.81175600	-1.87264300	-1.16155000
H	-2.41925700	-2.78137600	-0.69042400
C	-2.83979500	-1.05818900	1.67773000
H	-3.93120400	-0.96643900	1.64260000
C	-2.29336700	-0.10445800	2.74887400
H	-2.75263900	-0.32960200	3.71927400
H	-1.20907800	-0.22701000	2.85086900
H	-2.49198300	0.94699500	2.51864200
C	-2.48631900	-2.50999000	2.02298600
H	-1.40809700	-2.68666100	1.95210600
H	-2.79928700	-2.72691100	3.05193300
H	-2.98909700	-3.22751000	1.36762900
C	-2.15772300	-1.78565600	-2.54848500
H	-2.37308600	-2.70231100	-3.11185300
H	-2.53786500	-0.94217900	-3.13106200
H	-1.06995200	-1.68426300	-2.47027900
C	-4.33622800	-1.99359500	-1.25556300
H	-4.60214400	-2.89097100	-1.82883600
H	-4.80706800	-2.07730600	-0.27052600
H	-4.77298800	-1.13172000	-1.77021300
C	-2.91617100	1.45577200	-1.83122200
H	-3.62416800	0.87334000	-2.42947000
H	-3.16176200	2.51641600	-1.96306800
H	-1.91176900	1.29421400	-2.23181600
C	-4.44971900	1.24697300	0.16842600
H	-4.52047900	1.12572600	1.25305600
H	-4.80505500	2.25754000	-0.07060100
H	-5.13646200	0.53614300	-0.30022800

TS2-THF:

E: -1895.981716

G293: -1895.445081

G243: -1895.429782

Pd	-0.25975500	-0.67234100	-0.28913100
C	0.55785600	3.95946200	-1.28565600
C	0.53922100	3.02967900	-2.31690600
C	0.29894900	1.68753300	-2.00516700
C	0.06142900	1.26688800	-0.68507700
C	0.08674500	2.24516700	0.32207300
C	0.33945700	3.59214300	0.03450500
H	0.71849900	3.35132100	-3.33861900
H	0.30653600	0.96178700	-2.81340700
H	-0.09875100	1.97100800	1.35446400
H	0.36256900	4.34435400	0.81771200
O	-0.30671800	-2.84047100	0.20374600
B	0.79303800	-2.45412100	0.71518000
O	1.74398400	-2.66750600	1.61627300
H	2.25714500	-1.87014400	1.92534200
C	4.20820600	-1.34536900	-2.10613800
C	4.04455600	-0.34901100	-1.14784100
C	2.80132600	-0.21860400	-0.53234900

C	1.71895500	-1.06532800	-0.84446800
C	1.94106800	-2.05458600	-1.82373000
C	3.17845100	-2.20243500	-2.46227500
H	4.87468200	0.30826700	-0.90654000
H	2.66468700	0.57516600	0.19160700
H	1.13905000	-2.73654100	-2.09249900
F	0.79868100	5.26634200	-1.57765000
F	5.41513000	-1.47787700	-2.71125400
H	3.34419400	-2.96529800	-3.21685500
P	-2.57705900	-0.34576800	0.08683900
C	-3.29550100	1.25667800	-0.55690600
H	-2.56563300	1.99437900	-0.20380700
C	-3.44536000	-1.81955800	-0.66662100
H	-3.05464700	-2.63587000	-0.04831800
C	-3.06891200	-0.38941500	1.88862900
H	-4.15635700	-0.25751400	1.92745600
C	-2.40454100	0.76526700	2.65007100
H	-2.77110100	0.78631300	3.68363300
H	-1.31922000	0.62952300	2.68272700
H	-2.60969400	1.74228600	2.20195200
C	-2.71628100	-1.73334500	2.53833700
H	-1.65319400	-1.96643700	2.42046000
H	-2.94016800	-1.69029000	3.61148700
H	-3.28974000	-2.56275400	2.11395400
C	-2.97800300	-2.09945700	-2.10279300
H	-3.33243300	-3.09015200	-2.41396700
H	-3.37248800	-1.36805900	-2.81332400
H	-1.88563700	-2.09335100	-2.17472900
C	-4.97386900	-1.81435700	-0.56008300
H	-5.36652300	-2.79389300	-0.86136700
H	-5.32120400	-1.61746600	0.45933000
H	-5.41717200	-1.06443700	-1.22299400
C	-3.28070900	1.29743500	-2.09103700
H	-4.08252700	0.68206700	-2.51128800
H	-3.43938800	2.32792400	-2.43101600
H	-2.32859500	0.95284000	-2.50339500
C	-4.67340100	1.65274900	-0.01105900
H	-4.68432300	1.73824700	1.07910700
H	-4.94978900	2.63373600	-0.41821400
H	-5.45178500	0.94304400	-0.30486400
C	3.79620800	0.38245000	2.75136200
O	2.69824300	-0.55609300	2.84141000
C	1.46829400	0.14123000	3.15619200
C	1.88965800	1.54271200	3.58910400
C	3.15724900	1.77073100	2.75274300
H	4.44352300	0.23582500	3.62501200
H	4.36658000	0.15653800	1.84701500
H	0.84462400	0.16339200	2.25425400
H	0.94603500	-0.42445500	3.93353000
H	1.10997200	2.28534200	3.39828400
H	2.12718200	1.55703600	4.65869800
H	2.88707200	2.07616100	1.73597600
H	3.82273800	2.52931300	3.17397800

14:

E: -1739.932313

G293: -1739.483307

G243: -1739.469285

Pd	0.27507500	-0.33243300	-0.21704700
C	0.20447700	1.63800800	0.01755600
C	0.24030300	2.50845800	-1.08361300
C	0.10379600	2.20179800	1.30030200
C	0.15118200	3.89486600	-0.92009700
H	0.33402500	2.10925200	-2.08969200
C	0.01649600	3.58660000	1.48450700

H	0.07959200	1.56093900	2.17775300	C	-1.78540800	4.04003700	-0.06650700
C	0.03687700	4.40778200	0.36521700	H	-1.18359900	2.73599600	1.51873300
H	0.17255200	4.56919800	-1.77111700	C	-1.80788600	4.22778300	-1.44158000
H	-0.06975400	4.02359400	2.47497800	H	-1.27296000	3.49231900	-3.38628800
C	2.32801700	-0.12447400	-0.23831000	H	-2.22724400	4.78523200	0.58857700
C	3.04263600	-0.77431000	-1.26746800	C	1.98998500	1.16726100	0.20451400
C	3.09250700	0.58165300	0.71025500	C	3.10348300	0.50886900	-0.35788600
C	4.43702600	-0.72674000	-1.35423600	C	2.23361200	2.42931400	0.77972000
H	2.50440700	-1.34368900	-2.02169700	C	4.38768000	1.06624500	-0.34565500
C	4.49110300	0.63022200	0.65803300	H	2.98965200	-0.47126500	-0.81199900
H	2.59399300	1.11919600	1.51277100	C	3.50944200	3.00303600	0.81936700
C	5.13629200	-0.02420200	-0.38076900	H	1.41048500	2.99511100	1.20815500
H	4.97795300	-1.22562000	-2.15329800	C	4.56618800	2.30649800	0.25034200
H	5.07153000	1.17012400	1.40057700	H	5.23674200	0.54950100	-0.78434200
F	6.49370900	0.02193300	-0.44973000	H	3.68462900	3.97367300	1.27484000
F	-0.05424400	5.75521400	0.53295300	F	5.81178700	2.85599500	0.27493200
P	-2.13899100	-0.41890000	-0.20059300	F	-2.39011100	5.34976200	-1.94651800
C	-2.97591100	0.96916000	-1.17952500	P	-2.04924700	-0.75509800	0.50675100
H	-2.25165400	1.18219200	-1.97492000	C	-3.17271300	-0.54876300	-1.00510800
C	-2.77385200	-0.24082100	1.54987600	H	-2.46735800	-0.59672300	-1.84458300
H	-2.57722900	0.81571700	1.76645300	C	-2.94369900	0.11740900	1.90274900
C	-2.89051200	-1.97737100	-0.92191400	H	-3.15675900	1.10099800	1.46930400
H	-3.96620900	-1.79824800	-1.01758000	C	-2.13831200	-2.59061400	0.86733100
C	-2.70967200	-3.22267200	-0.04383400	H	-3.19964500	-2.86106100	0.85709200
H	-3.04039300	-4.10976600	-0.59852700	C	-1.56165700	-2.96913100	2.23740200
H	-1.67127200	-3.38713500	0.25399700	H	-1.54040000	-4.06279500	2.33091600
H	-3.30366700	-3.16707500	0.87113500	H	-0.53781000	-2.60519000	2.35325900
C	-2.31488800	-2.20257200	-2.32914100	H	-2.16416500	-2.58175900	3.06222200
H	-1.23978700	-2.41404800	-2.30169200	C	-1.41677600	-3.37187000	-0.24139500
H	-2.81058100	-3.05670500	-2.80589400	H	-0.33857300	-3.22186900	-0.17312500
H	-2.44500400	-1.33226200	-2.97965900	H	-1.61518100	-4.44513100	-0.12863000
C	-3.14232700	2.25056100	-0.34747300	H	-1.73328700	-3.07919700	-1.24667000
H	-3.40891000	3.07803700	-1.01576800	C	-3.84852900	0.83103000	-1.04379900
H	-3.95234500	2.14332000	0.38207600	H	-4.30069900	0.98119400	-2.03175200
H	-2.23570800	2.53325800	0.18649800	H	-4.65237500	0.89529700	-0.30240900
C	-4.31731200	0.61462000	-1.83762100	H	-3.15380700	1.65133300	-0.86718000
H	-4.69079500	1.49569600	-2.37458100	C	-4.23651100	-1.63703600	-1.21512700
H	-4.23797600	-0.19766300	-2.56423800	H	-4.79778700	-1.41137500	-2.13083700
H	-5.07473300	0.33774000	-1.09710800	H	-3.81312300	-2.63715400	-1.33203400
C	-4.27433100	-0.49499900	1.73352300	H	-4.95599000	-1.66780500	-0.39089900
H	-4.54216100	-1.53422200	1.51730100	C	-4.27186600	-0.51568400	2.33169500
H	-4.55977700	-0.29147400	2.77357500	H	-4.13118700	-1.52159200	2.74080200
H	-4.88062100	0.14970500	1.09129500	H	-4.73700100	0.09565100	3.11581100
C	-1.92220700	-1.05848400	2.53291900	H	-4.98114300	-0.58350900	1.50239900
H	-0.85713300	-0.83042900	2.41596600	C	-2.01348000	0.35808900	3.10195200
H	-2.21307500	-0.81702400	3.56313000	H	-1.07002400	0.81582400	2.78497100
O	-2.05096000	-2.13612500	2.39613300	H	-2.49979800	1.03412000	3.81663500
H	0.62597300	-2.58911400	-0.35925300	H	-1.77299800	-0.56768900	3.63217400
B	1.14446100	-3.24422500	0.76002600	O	1.25555600	-1.65831200	0.91042700
O	0.80294700	-4.55502300	0.93115900	B	2.14287700	-1.62556900	1.96873300
H	1.21850400	-4.92816300	1.72536700	O	3.12587400	-2.57416800	2.03404000
O	1.94335300	-2.57159200	1.62674800	H	3.69987400	-2.42283900	2.80186700
H	2.10571300	-1.65934500	1.30986700	O	1.98912200	-0.68689800	2.95259400
H	0.03902900	-3.15343100	-0.88754400	H	1.37973700	0.00944900	2.64694900
14-THF:				H	1.55800400	-2.13696800	0.08843200
E: -1972.517781				C	1.14450300	-1.92280300	-2.48431000
G293: -1971.954334				O	1.89277600	-2.61699100	-1.45026800
G243: -1971.938452				C	2.02534100	-4.02062800	-1.78264400
Pd	0.16113300	0.21175400	0.28077300	C	1.00970100	-4.27610000	-2.89251900
C	-0.62987700	1.90729900	-0.40336200	C	0.99231400	-2.92684800	-3.62686700
C	-0.65693500	2.15420100	-1.78763300	H	0.17837500	-1.62040200	-2.06491800
C	-1.19037200	2.87946800	0.44201800	H	1.70123500	-1.02390600	-2.76073900
C	-1.24797200	3.30624300	-2.31657200	H	3.05258200	-4.19974600	-2.12291800
H	-0.21447600	1.43825300	-2.47530900	H	1.84755000	-4.60110800	-0.87320500
				H	1.30259100	-5.11148900	-3.53447300
				H	0.02514900	-4.49489200	-2.46635100
				H	1.84407500	-2.85618000	-4.31241800

H 0.07563700 -2.75934900 -4.19936400

15:

E: -1663.395147

G293: -1662.974107

G243: -1662.960359

Pd	-0.24824400	-0.47345100	-0.08767800
C	-0.22973800	1.51850800	-0.02341300
C	-0.29073000	2.19255800	1.20683100
C	-0.11028800	2.28923900	-1.19133300
C	-0.20301100	3.58685700	1.28072100
H	-0.39853300	1.63256000	2.13146000
C	-0.02514500	3.68514500	-1.13758600
H	-0.07291600	1.80628100	-2.16273800
C	-0.06767200	4.30791700	0.10244600
H	-0.23951300	4.10770200	2.23292000
H	0.06940000	4.28172700	-2.04011300
C	-2.29405100	-0.34779500	-0.12490100
C	-3.08014100	0.15890200	0.93330700
C	-2.99082800	-0.87140700	-1.23480200
C	-4.47976600	0.12460600	0.90603300
H	-2.59524600	0.59664500	1.80264400
C	-4.38908200	-0.89871100	-1.29512600
H	-2.43520400	-1.27969600	-2.07622200
C	-5.10771300	-0.40385700	-0.21630300
H	-5.07675300	0.50866600	1.72789800
H	-4.91525400	-1.30423200	-2.15416200
F	-6.46353800	-0.43855300	-0.25422600
F	0.02105500	5.66426200	0.16441600
O	-0.43786800	-2.85369100	-0.02272900
B	-1.42605400	-2.70317800	0.71300700
O	-2.41339000	-2.82933000	1.57754800
H	-2.97215900	-2.02388200	1.61544300
P	2.13545300	-0.64385300	-0.12754400
C	2.73526700	-1.09839400	-1.83739900
H	3.83100300	-1.10069400	-1.81875100
C	3.07230300	0.92211600	0.29488400
H	2.47852200	1.69220200	-0.21089300
C	2.70163900	-2.05638600	0.95898100
H	2.25199900	-2.91567000	0.44860700
C	2.25315500	-0.04144400	-2.84127000
H	2.66661900	-0.25351500	-3.83494900
H	1.15993200	-0.05919500	-2.91813100
H	2.55288600	0.97372400	-2.56250700
C	2.25026400	-2.49188700	-2.25642900
H	1.16082000	-2.57378100	-2.17874400
H	2.53202000	-2.67866600	-3.30024900
H	2.69317200	-3.28658800	-1.64844000
C	3.01744500	1.21644500	1.80017500
H	3.69641900	0.56209500	2.35622900
H	3.32978200	2.25185400	1.98209900
H	2.01069400	1.09635400	2.20894200
C	4.51144000	1.01544000	-0.22796000
H	4.56527200	0.93719400	-1.31734200
H	4.93044500	1.99103000	0.05022600
H	5.15722700	0.24431300	0.20181000
C	2.07144900	-2.00480300	2.35887300
H	2.23677100	-2.96169400	2.86977300
H	2.51026500	-1.21860200	2.97906100
H	0.99145700	-1.83194500	2.30591000
C	4.21731700	-2.27047100	1.02719200
H	4.43526200	-3.21601000	1.54023000
H	4.67504600	-2.31867300	0.03368700

15-THF:

E: -1895.985914

G293: -1895.450095

G243: -1895.434611

Pd	-0.09008600	-0.35883100	0.62668200
C	-0.06145000	1.60753600	0.29492200
C	0.05035400	2.12308400	-1.00776200
C	-0.15173500	2.53003800	1.35133400
C	0.05027100	3.49968100	-1.25857200
H	0.13363100	1.45163800	-1.85486900
C	-0.15781300	3.91048100	1.12236500
H	-0.21568900	2.17871200	2.37623900
C	-0.05893900	4.37061600	-0.18373100
H	0.13278500	3.89148400	-2.26822400
H	-0.22982000	4.61957200	1.94189800
C	1.91008000	-0.22234900	1.12762000
C	2.86744700	0.60376500	0.50834400
C	2.37293600	-1.02926600	2.18946000
C	4.21293700	0.61122500	0.89052600
H	2.56337000	1.27232900	-0.29058400
C	3.71144300	-1.03374600	2.60110800
H	1.68051700	-1.68340000	2.71349300
C	4.61017700	-0.21416400	1.93430500
H	4.94237100	1.24724100	0.39685200
H	4.05380500	-1.65836900	3.42124600
F	5.91582100	-0.21329000	2.31716700
F	-0.06436200	5.71169300	-0.41586200
O	-0.04138200	-2.67196900	0.98943100
B	0.89064200	-2.85423000	0.18464900
O	1.83166100	-3.20735600	-0.63041200
H	2.05733300	-2.59046900	-1.43403200
P	-2.45738000	-0.52593500	0.27377300
C	-3.31794300	-0.54923300	1.93436700
H	-4.39791800	-0.55422500	1.74869900
C	-3.25317400	0.90509100	-0.63645200
H	-2.69929500	1.76429700	-0.24205800
C	-2.96762100	-2.15001800	-0.50708500
H	-2.63121500	-2.86778100	0.24929200
C	-2.95256700	0.71400600	2.72580200
H	-3.54216900	0.75773300	3.65000000
H	-1.89269400	0.69679100	3.00036000
H	-3.13727600	1.63537300	2.16476200
C	-2.95546300	-1.80174100	2.74241600
H	-1.87068300	-1.89544900	2.86099400
H	-3.40233600	-1.73358300	3.74226200
H	-3.32608100	-2.72039500	2.27767500
C	-2.97112400	0.83039500	-2.14332900
H	-3.60776800	0.08255600	-2.62694500
H	-3.18590800	1.80068200	-2.60724700
H	-1.92818300	0.58151800	-2.35933600
C	-4.74488700	1.14578800	-0.37269900
H	-4.95731300	1.32367900	0.68520900
H	-5.06588300	2.03902200	-0.92415500
H	-5.36480100	0.31009400	-0.70925600
C	-2.18250800	-2.47019000	-1.78587500
H	-2.37693200	-3.50832800	-2.08372400
H	-2.46986700	-1.82704500	-2.62202600
H	-1.10669500	-2.36278900	-1.63129800
C	-4.47454700	-2.33452400	-0.71752400
H	-4.68316100	-3.37416900	-1.00111500
H	-5.05277000	-2.11502800	0.18567100
H	-4.84493900	-1.69310700	-1.52366300
C	3.40179100	-0.86592200	-2.74140800
O	2.26235400	-1.77352300	-2.64766100
C	1.05176700	-1.09942500	-3.08534000

C	1.54767300	0.02978800	-3.97708500
C	2.83666000	0.45812200	-3.25945700
H	3.86154200	-0.78388900	-1.75382100
H	4.11317800	-1.31876600	-3.43897700
H	0.43045900	-1.83998700	-3.59412400
H	0.52201600	-0.72154700	-2.20168000
H	1.76701800	-0.34864700	-4.98156000
H	0.81716100	0.83913000	-4.06221200
H	3.54315100	0.97211200	-3.91646800
H	2.59574200	1.12235600	-2.42461600

16:

E: -1487.288122

G293: -1486.886291

G243: -1486.873708

Pd	0.31526600	-0.52899200	0.03890500
C	0.45556400	1.44376100	0.03313200
C	0.04022800	2.18256300	-1.08462700
C	0.93172200	2.13620500	1.15799400
C	0.07992700	3.58161300	-1.07890800
H	-0.32817800	1.67757400	-1.97147000
C	0.96637900	3.53446400	1.18065700
H	1.27929300	1.59182700	2.02995700
C	0.53808200	4.23144400	0.05880000
H	-0.24080400	4.15918000	-1.94078100
H	1.32609600	4.07648000	2.05008900
C	2.33866800	-0.68885400	0.01021900
C	3.32767200	0.20839800	-0.43060500
C	2.76876900	-1.96548300	0.42688600
C	4.68057500	-0.14514300	-0.46500900
H	3.04765900	1.20662700	-0.75504500
C	4.11620400	-2.34357600	0.40334900
H	2.04089300	-2.69717400	0.78173400
C	5.04794700	-1.41715800	-0.04504000
H	5.44233000	0.54757900	-0.81113400
H	4.44195000	-3.32764900	0.72753200
F	6.36219400	-1.76665700	-0.07291700
F	0.57286600	5.59069600	0.07314800
P	-2.08630100	-0.67916500	0.01400700
C	-3.05223200	0.90827200	0.20602400
H	-2.61855600	1.55601400	-0.56521100
C	-2.70769900	-1.83776700	1.35578500
H	-2.92297100	-1.16905800	2.19810000
C	-2.63695000	-1.40534900	-1.61542200
H	-3.70541500	-1.63947500	-1.54945400
C	-1.85557000	-2.69709800	-1.89508500
H	-2.14773200	-3.10920600	-2.86899600
H	-0.77622500	-2.49716700	-1.92554600
H	-2.03574100	-3.46698000	-1.13958600
C	-2.41532700	-0.39803700	-2.75147800
H	-1.35371100	-0.13964200	-2.83984700
H	-2.73149700	-0.84054800	-3.70419800
H	-2.98187600	0.52728800	-2.60975900
C	-2.76233700	1.55781100	1.56567000
H	-3.19390300	2.56578000	1.59102800
H	-3.21210200	0.98845300	2.38710100
H	-1.68912800	1.64641600	1.75431800
C	-4.56077500	0.79385800	-0.03950600
H	-5.01055200	1.79481700	-0.03246200
H	-4.79680200	0.33167400	-1.00300300
H	-5.04870000	0.21050900	0.74839200
C	-3.98599300	-2.61649800	1.02150700
H	-3.81559200	-3.34709400	0.22385900
H	-4.31811800	-3.17168600	1.90784900
H	-4.80569100	-1.96298800	0.71181300

C	-1.57915900	-2.78371900	1.79613900
H	-0.69077300	-2.22271300	2.10992200
H	-1.90870100	-3.40010400	2.64214800
H	-1.28288500	-3.46223100	0.98796100

TS3:

E: -1487.272576

G293: -1486.871386

G243: -1486.858903

Pd	0.20819200	-0.62930200	0.08931500
C	1.12218700	1.20546400	-0.04043400
C	1.08087900	1.84415600	-1.29392900
C	1.18569900	2.00520300	1.11536000
C	1.03493600	3.23647200	-1.39145100
H	1.06854600	1.25511600	-2.20561500
C	1.14374000	3.39857900	1.03049800
H	1.25572100	1.54314700	2.09499100
C	1.06097200	3.98982800	-0.22425900
H	0.98157400	3.73389400	-2.35506000
H	1.17534200	4.01992200	1.92030700
C	2.25931900	-0.50717100	0.05193500
C	2.90496300	-0.86336700	-1.14719300
C	2.92593900	-0.74506900	1.26888700
C	4.15616900	-1.48287900	-1.13579600
H	2.43373300	-0.65147000	-2.10277200
C	4.17694300	-1.36491200	1.29649300
H	2.47105900	-0.44137500	2.20753800
C	4.76680400	-1.72355600	0.08985200
H	4.65845900	-1.76925000	-2.05471100
H	4.69422300	-1.56283700	2.23030100
F	5.98667300	-2.31646600	0.10824400
F	1.01595100	5.34497300	-0.31309500
P	-2.15065700	-0.71859000	0.00761600
C	-2.81292000	0.79552300	-0.88769300
H	-2.14260900	0.84553700	-1.75569000
C	-2.98813400	-0.89332900	1.67572100
C	-2.80015500	-2.16212900	-0.98738300
H	-3.89481300	-2.10506200	-1.01738300
C	-2.39271400	-3.49061100	-0.33681800
H	-2.70071500	-4.32891900	-0.97402300
H	-1.30345800	-3.54722500	-0.21133000
H	-2.85486500	-3.63556100	0.64453700
C	-2.25198400	-2.08564400	-2.41967700
H	-1.15495000	-2.11748800	-2.41371200
H	-2.61218000	-2.94008700	-3.00593900
H	-2.55703200	-1.17226100	-2.93956200
C	-2.58377100	2.07139600	-0.06601900
H	-2.75208700	2.95220200	-0.69788800
H	-3.28222900	2.13135400	0.77535700
H	-1.56504300	2.12946800	0.32699300
C	-4.25392800	0.72713500	-1.40955100
H	-4.45522400	1.61222000	-2.02703500
H	-4.43544300	-0.15341600	-2.03267600
H	-4.98359100	0.72203100	-0.59594800
C	-4.51042200	-0.71981600	1.69044500
H	-5.00446300	-1.32202300	0.92087700
H	-4.90999700	-1.03047300	2.66445700
H	-4.79223500	0.32698600	1.53905100
C	-2.30813900	-0.01737400	2.73833300
H	-2.47370500	1.04875800	2.55688200
H	-2.71364300	-0.25418700	3.73036000
H	-1.22659700	-0.19069600	2.75898600
H	-2.76268300	-1.93552900	1.93570600

18:

E: -662.0962952

G293: -661.9628892

G243: -661.9558972

C	-2.85650500	-1.15733300	-0.37097900
C	-1.46300800	-1.14802900	-0.37005200
C	-0.74126200	-0.00002800	-0.00007300
C	-1.46294100	1.14798600	0.37001000
C	-2.85643200	1.15736100	0.37096300
C	-3.52925400	0.00004400	-0.00004600
H	-3.41754100	-2.03888500	-0.66336600
H	-0.93012900	-2.04049300	-0.68292300
H	-0.92999600	2.04041100	0.68288300
H	-3.41742600	2.03891000	0.66344000
C	0.74126200	-0.00004400	-0.00009700
C	1.46297000	1.14798100	-0.37009000
C	1.46297800	-1.14801800	0.37002300
C	2.85646200	1.15734400	-0.37096400
H	0.93005200	2.04043200	-0.68293100
C	2.85647500	-1.15736300	0.37093400
H	0.93007400	-2.04045400	0.68293100
C	3.52925500	-0.00001800	-0.00004500
H	3.41747900	2.03891800	-0.66332400
H	3.41748800	-2.03890000	0.66341100
F	-4.88378900	0.00003300	0.00013300
F	4.88378900	0.00005100	0.00013100

8:

E: -2464.325886

G293: -2463.620676

G243: -2463.602447

Pd	-1.56615600	0.10026800	0.61516600
O	-0.04198800	1.34433900	1.46183700
Pd	1.54053900	0.14103000	0.64970200
O	0.00424500	-1.39166400	1.00554000
C	2.63823100	1.76824400	0.24830500
C	2.18901400	2.61316400	-0.78627200
C	3.74650200	2.19674800	0.99764300
C	2.82337200	3.82560600	-1.07614200
H	1.33410100	2.32149600	-1.39164900
C	4.39597300	3.40668600	0.72472400
H	4.12426500	1.58602100	1.81167000
C	3.92314700	4.19682800	-0.31354800
H	2.47624900	4.47225500	-1.87674300
H	5.25404200	3.73353400	1.30490600
C	-2.80366400	1.64171900	0.29571700
C	-2.82500300	2.34303200	-0.92383900
C	-3.60724400	2.13543400	1.34042700
C	-3.61932700	3.48157600	-1.10534500
H	-2.21716500	2.00299100	-1.75693400
C	-4.41089700	3.26929500	1.17951900
H	-3.61410600	1.63173400	2.30363400
C	-4.40316800	3.92009100	-0.04710500
H	-3.63179800	4.02147400	-2.04778000
H	-5.03241200	3.64498900	1.98713600
F	-5.18454700	5.02161800	-0.21535400
F	4.55285800	5.37038700	-0.59076000
P	-2.99119000	-1.41594100	-0.28764600
P	3.13610700	-1.25897400	-0.16162300
C	-4.76614100	-0.88074500	-0.53339400
C	-2.41562900	-1.93338600	-1.98687200
C	-2.89086400	-2.97567900	0.73357200
C	-2.34219700	-0.71014700	-2.91034600
H	-1.54724000	-0.03279200	-2.57974100
H	-2.11081100	-1.03133600	-3.93332900

H	-3.27881300	-0.14434800	-2.93918800
C	-3.73978800	-4.14405900	0.22121500
H	-3.57689100	-4.34498500	-0.84263200
H	-3.48108500	-5.05569900	0.77473400
H	-4.80772900	-3.95826600	0.37445600
C	3.59608900	-1.00567200	-1.95463200
H	4.12810100	-1.91448400	-2.25672500
C	2.45558200	-3.00581300	-0.10255500
C	4.75580900	-1.15581500	0.75797600
C	2.31685600	-0.88354900	-2.79269100
H	1.65965500	-1.74942900	-2.67094100
H	1.74913700	0.00898600	-2.50749200
H	2.57267900	-0.80193900	-3.85644200
C	4.53206300	0.18458200	-2.19529200
H	4.08299200	1.12582000	-1.87075300
H	5.49290600	0.06691800	-1.68558200
H	4.73822300	0.26198200	-3.27035400
C	3.06583600	-4.00496400	-1.09325800
H	2.57634000	-4.97837300	-0.96009900
H	2.91382500	-3.70592100	-2.13425900
H	4.13818200	-4.15131000	-0.93175400
H	-0.04263900	2.22724200	1.05717200
H	-0.02085100	-1.49137600	1.97199700
C	2.46653600	-3.56805000	1.32470800
H	3.47405700	-3.86500000	1.63317400
H	2.07729400	-2.84853300	2.04982200
H	1.83077800	-4.46119600	1.36487400
H	1.40625300	-2.84538000	-0.36498600
H	5.11388100	-0.16161200	0.46757300
C	4.57740800	-1.13961200	2.28339300
H	3.75535800	-0.48376300	2.58852200
H	4.37415500	-2.13787200	2.67884200
H	5.49914900	-0.77665500	2.75460000
C	5.79987700	-2.19067900	0.32298900
H	6.76150900	-1.96584100	0.80135100
H	5.50817500	-3.20084700	0.62664700
H	5.96003200	-2.19138400	-0.75976100
H	-4.65170400	0.14110800	-0.91143700
C	-1.05766100	-2.64282200	-1.93466000
H	-0.31469500	-2.01980300	-1.43078100
H	-1.10817300	-3.60140300	-1.40969300
H	-0.71150200	-2.84147600	-2.95661200
H	-3.16506000	-2.63119200	-2.37719200
H	-1.83036200	-3.22540600	0.61760400
C	-3.11745700	-2.72489700	2.23141700
H	-2.79617400	-3.60705700	2.79940500
H	-2.54064200	-1.86379000	2.58495900
H	-4.17057800	-2.54684800	2.46480600
C	-5.51620200	-0.79910800	0.80266400
H	-6.44565900	-0.23369800	0.66504300
H	-5.78464600	-1.79613400	1.16621500
H	-4.93023300	-0.29593000	1.57624200
C	-5.57003600	-1.68182900	-1.56593600
H	-6.57881400	-1.25599600	-1.63846200
H	-5.12601800	-1.63879600	-2.56432400
H	-5.67586400	-2.73314800	-1.28286900

8-THF:

E: -2696.903575

G293: -2696.084053

G243: -2696.063927

Pd	1.51597700	-0.39260400	0.62058200
O	0.02262300	0.94150200	1.31557800
Pd	-1.60584900	-0.20141200	0.57358500
O	-0.14217600	-1.71260000	1.20410100

C	-2.67608000	1.42835000	0.09631000
C	-3.09798100	2.28778300	1.12827500
C	-2.95167700	1.82432100	-1.22357800
C	-3.78527900	3.47647400	0.86476300
H	-2.89141800	2.03097800	2.16368800
C	-3.63840000	3.00994800	-1.51231100
H	-2.62913800	1.20837000	-2.05683600
C	-4.04884200	3.81226400	-0.45737400
H	-4.11196100	4.13385300	1.66528100
H	-3.84946900	3.30971400	-2.53479700
C	2.82183100	1.05784400	0.17299000
C	3.83133600	1.45683200	1.06741500
C	2.70948700	1.77016800	-1.03461600
C	4.70185700	2.51443200	0.77426800
H	3.95462100	0.93575800	2.01323500
C	3.57433700	2.82313400	-1.35312100
H	1.93512800	1.50401000	-1.74940200
C	4.55713300	3.17580600	-0.43758100
H	5.47872300	2.82091600	1.46870200
H	3.49073000	3.36407100	-2.29088500
F	5.40103400	4.20146400	-0.73713500
F	-4.72568000	4.96291200	-0.72482900
P	2.94835600	-2.03601400	-0.05102500
P	-3.30541700	-1.58821400	-0.05453600
C	4.56544800	-1.51342000	-0.84087600
C	3.46236900	-3.07728000	1.41231700
C	2.04297800	-3.22358400	-1.17988200
C	4.11677900	-2.17251200	2.46590100
H	3.38224100	-1.46776100	2.87176500
H	4.50085400	-2.78101400	3.29381500
H	4.95218600	-1.59235600	2.06015900
C	2.88506300	-4.39438800	-1.69946600
H	3.40959700	-4.91848900	-0.89413000
H	2.23264800	-5.12056000	-2.20073200
H	3.62728100	-4.05860300	-2.42995600
C	-4.90286300	-1.35458600	0.88670800
H	-5.49270100	-2.25930000	0.70420300
C	-2.81263700	-3.35782700	0.35171000
C	-3.79275500	-1.46109900	-1.85128900
C	-4.59168200	-1.26103500	2.38672000
H	-4.01323400	-2.11926000	2.74579400
H	-4.01420000	-0.35611800	2.60435700
H	-5.52533500	-1.21959500	2.96117600
C	-5.73419500	-0.15441900	0.41870200
H	-5.19465000	0.78620200	0.54712300
H	-6.03317400	-0.24042800	-0.63035100
H	-6.65131400	-0.10267500	1.01912000
C	-3.95945200	-4.34581100	0.60302400
H	-3.53402800	-5.33464900	0.81701900
H	-4.57060200	-4.06263200	1.46409000
H	-4.61541800	-4.44974000	-0.26628800
H	0.07213200	1.86267400	0.98675600
H	-0.17489200	-2.50166000	0.64615200
C	-1.83334600	-3.92670600	-0.68612500
H	-2.35753800	-4.23783200	-1.59504500
H	-1.06453000	-3.20867900	-0.98209100
H	-1.33377400	-4.81166200	-0.27342200
H	-2.26536000	-3.23229300	1.29286400
H	-4.23609100	-0.45986100	-1.88888900
C	-2.58212200	-1.45218400	-2.79709800
H	-1.77010300	-0.82723200	-2.41145300
H	-2.18478100	-2.45750300	-2.95645600
H	-2.88501700	-1.05726600	-3.77481700
C	-4.85489800	-2.47071200	-2.30209500
H	-5.18481500	-2.22629600	-3.31976100
H	-4.45602100	-3.48968300	-2.32010200
H	-5.73808400	-2.46107100	-1.65567700

H	4.84453000	-0.63741700	-0.24630200
C	2.28141300	-3.84763200	2.01610500
H	1.45274100	-3.17492000	2.26106600
H	1.90633400	-4.62071900	1.33717900
H	2.60649300	-4.34870100	2.93654700
H	4.20232300	-3.79981400	1.05090400
H	1.27833900	-3.63534400	-0.51053000
C	1.29980600	-2.50652300	-2.31643800
H	0.62361500	-3.21225000	-2.81409500
H	0.70437700	-1.66897700	-1.93894200
H	1.98793300	-2.11915100	-3.07223000
C	4.36692500	-1.04204200	-2.28789100
H	5.26861200	-0.51599700	-2.62401500
H	4.20513100	-1.88845600	-2.96265000
H	3.52462200	-0.35358900	-2.38624600
C	5.71411200	-2.52762600	-0.75210600
H	6.60417400	-2.09387200	-1.22538700
H	5.98037000	-2.76796800	0.28075100
H	5.48632700	-3.46153600	-1.27359200
C	-0.17976900	4.12246100	-0.65494800
O	0.13051900	3.67720800	0.68057600
C	1.28408000	4.37948600	1.17244200
C	1.31060500	5.69107900	0.39297600
C	0.82147400	5.23824700	-0.99182600
H	-0.10933200	3.27270700	-1.34266800
H	-1.21489900	4.47847800	-0.65352000
H	1.15829200	4.50663100	2.25216800
H	2.18775900	3.78785100	0.98923200
H	0.61038900	6.40986100	0.83445000
H	2.30630400	6.14442200	0.36933000
H	0.36136600	6.04418400	-1.57109000
H	1.65949600	4.83664500	-1.56922900

20:**E: -2972.092280****G293: -2971.274232****G243: -2971.253413**

Pd	1.04248200	0.82987300	-0.23302600
O	-0.31470600	0.62510500	-1.86271200
Pd	-1.57423800	-0.59480300	-0.65685600
O	0.64420600	-1.40567400	-0.68462000
C	-3.04648800	0.67780100	-1.01625900
C	-2.93926100	1.95943400	-0.45147000
C	-4.07618900	0.42980000	-1.93289000
C	-3.85437000	2.96673500	-0.77013700
H	-2.13609000	2.18617200	0.24126400
C	-5.00298900	1.42711900	-2.25849700
H	-4.17163600	-0.54166000	-2.40621700
C	-4.87749400	2.67526000	-1.66372200
H	-3.77488800	3.95989300	-0.33861800
H	-5.80788100	1.24250500	-2.96346300
C	0.91201200	2.80664400	-0.33052200
C	0.24374500	3.59857100	0.61448700
C	1.36363700	3.42018500	-1.51198700
C	0.02982900	4.96426800	0.39630000
H	-0.12378400	3.16168400	1.53533500
C	1.16440100	4.78517600	-1.74286800
H	1.87912500	2.83453100	-2.26806300
C	0.49894900	5.53246700	-0.77975400
H	-0.49239700	5.57819500	1.12403300
H	1.51634700	5.26296200	-2.65216500
F	0.29911300	6.85861700	-0.99656600
F	-5.77709900	3.64442200	-1.97236800
P	2.42982400	0.86886700	1.58554700
P	-2.98299600	-1.84033100	0.66036100

C	3.21298100	2.50195500	2.04215200
C	1.50507800	0.35407800	3.12334400
C	3.70979900	-0.46635400	1.33456600
C	0.51624500	1.42155100	3.60511600
H	-0.27299200	1.58374500	2.86488100
H	0.03493300	1.07832800	4.52909800
H	0.99466700	2.38202400	3.81872000
C	4.39179600	-1.00519700	2.59789800
H	3.67558400	-1.39101000	3.32875400
H	5.04593300	-1.83818300	2.31096300
H	5.01290800	-0.24974000	3.08844500
C	-3.87263600	-0.89947400	2.01566900
H	-4.23980600	-1.67115800	2.69961600
C	-2.02261200	-3.16876200	1.58796200
C	-4.35929900	-2.62092900	-0.32826300
C	-2.87554500	-0.01385800	2.77223500
H	-2.04139500	-0.58951400	3.18135100
H	-2.46208000	0.75575100	2.11361700
H	-3.38010300	0.48687400	3.60780600
C	-5.09167700	-0.09032100	1.55464700
H	-4.81964900	0.71076200	0.86616100
H	-5.85176700	-0.71445800	1.07663200
H	-5.55468700	0.36926600	2.43704300
C	-2.62893500	-3.61594300	2.92509500
H	-1.98284900	-4.38911200	3.35913000
H	-2.69545000	-2.80202400	3.65168300
H	-3.62528900	-4.05070600	2.79959600
H	-0.75715500	1.46639100	-2.06108300
H	0.57184300	-1.20433000	-1.63608400
C	-1.71979400	-4.38559900	0.70173400
H	-2.62420800	-4.96883400	0.50713100
H	-1.25481400	-4.11187900	-0.24925700
H	-1.02383500	-5.04830600	1.23390200
H	-1.07389400	-2.66685800	1.80459800
H	-4.95210700	-1.74418700	-0.61039000
C	-3.86522700	-3.26302900	-1.63244500
H	-3.16308200	-2.60981800	-2.16166800
H	-3.36321600	-4.21701900	-1.45539000
H	-4.72156800	-3.45290600	-2.29129600
C	-5.26767100	-3.56364000	0.47174000
H	-6.12475500	-3.85440200	-0.14848700
H	-4.74516600	-4.47939800	0.76270600
H	-5.66051500	-3.09289400	1.37837000
H	2.33216800	3.13945400	2.17560200
C	0.77525500	-0.96853200	2.86847000
H	-0.00227900	-0.82244400	2.11295400
H	1.42931300	-1.76090700	2.49955500
H	0.29580000	-1.31021700	3.79465100
H	2.26236900	0.20428300	3.90101000
H	3.10670500	-1.27736800	0.91424400
C	4.74584700	-0.06271500	0.27820200
H	5.27758400	-0.95600300	-0.06273600
H	4.28319900	0.40285700	-0.59702400
H	5.48487200	0.63060200	0.69044000
C	4.05210800	3.12720800	0.91895900
H	4.19280900	4.19420100	1.13050000
H	5.04247800	2.66992400	0.85538300
H	3.56900200	3.04142300	-0.05623600
C	3.99785100	2.48595100	3.36055100
H	4.28528800	3.51282700	3.61899600
H	3.41717300	2.08566500	4.19649900
H	4.91798600	1.90070700	3.27091800
B	1.38814200	-2.77841100	-0.69083100
C	2.86276500	-2.59944400	-1.35661900
C	3.94128100	-3.38926300	-0.92177600
C	3.11053800	-1.74458000	-2.44605100
C	5.20123800	-3.33971600	-1.52657600

H	3.78973300	-4.05758200	-0.07858300
C	4.35839100	-1.66523700	-3.07008900
H	2.31548500	-1.10934800	-2.83321200
C	5.38412500	-2.47119200	-2.59419900
H	6.02813300	-3.95483900	-1.18356900
H	4.53920700	-0.99780300	-3.90753300
O	0.49663000	-3.57421800	-1.55375600
H	0.96312100	-4.38279500	-1.81291100
O	1.52250000	-3.26379300	0.66208000
H	0.65757800	-3.58808500	0.94750500
F	6.60471000	-2.40729200	-3.19250800

TS4:**E: -2972.083518****G293: -2971.266202****G243: -2971.245464**

Pd	0.82154500	1.22698000	-0.36630400
O	-0.37341400	0.35994900	-1.95477300
Pd	-1.28693500	-0.99871800	-0.58571600
O	1.36013600	-0.91831100	-0.58814100
C	-3.02621200	-0.29289200	-1.21217800
C	-3.29158100	1.08128100	-1.09705400
C	-3.93466900	-1.09478400	-1.91730900
C	-4.44732400	1.64270000	-1.64794500
H	-2.60362200	1.73120400	-0.56863000
C	-5.09657800	-0.54723800	-2.47327500
H	-3.75257300	-2.15668700	-2.04139400
C	-5.33363100	0.81230300	-2.32140500
H	-4.65681000	2.70423600	-1.55644100
H	-5.80707100	-1.16302900	-3.01645400
C	0.06639000	3.05628600	-0.55013800
C	-0.96125900	3.53282000	0.28045400
C	0.44303700	3.84618600	-1.65054700
C	-1.59433200	4.75552500	0.03096500
H	-1.29255000	2.94672800	1.12985700
C	-0.17580600	5.07326500	-1.91342600
H	1.22562700	3.50721000	-2.32299900
C	-1.18431800	5.50588300	-1.06262300
H	-2.39354800	5.11989500	0.66959900
H	0.11526500	5.68403700	-2.76280500
F	-1.79032800	6.69696000	-1.31015100
F	-6.46342700	1.34660800	-2.85273000
P	2.32651800	1.85129100	1.22397300
P	-2.34267200	-2.08558900	1.15339300
C	2.87142700	3.63676900	1.15075300
C	1.75378600	1.60596500	2.98192900
C	3.76156800	0.66621600	1.03640500
C	0.57751900	2.52730600	3.32534700
H	-0.31971000	2.22091100	2.78298500
H	0.35990900	2.45538200	4.39802300
H	0.77176200	3.57851300	3.09260900
C	4.86372700	0.80298100	2.09385000
H	4.47400800	0.79545100	3.11636400
H	5.55589400	-0.04316600	1.99844300
H	5.44478000	1.72018400	1.95464500
C	-3.35311300	-0.91272600	2.21527900
H	-3.49493600	-1.43693500	3.16529000
C	-1.07526600	-2.80388200	2.35571600
C	-3.57434800	-3.39268300	0.64941500
C	-2.54420200	0.36378400	2.47866100
H	-1.56202300	0.14864900	2.90650900
H	-2.38615800	0.92010800	1.55088400
H	-3.08291400	1.01163700	3.18178500
C	-4.74909300	-0.57740700	1.67416500
H	-4.70802700	-0.06161100	0.71427900

H	-5.37926000	-1.46397300	1.56248400	O	-1.01163100	2.07337400	-0.87557000
H	-5.24747300	0.08894400	2.38988500	O	-2.19162900	-0.06105600	-1.21414500
C	-1.44619000	-2.69448500	3.84132600	O	0.48853900	-0.28864500	-1.88638800
H	-0.62799200	-3.12302300	4.43376300	H	-1.16684600	2.42720200	-1.76538200
H	-1.58175800	-1.66338900	4.17669100	H	-1.81963700	0.13248200	-2.09058300
H	-2.35466100	-3.25811500	4.08083400	H	1.32193100	-0.75586900	-2.06260000
H	-1.04963500	0.97307500	-2.28520800	C	-3.55352700	2.04061000	-0.56447100
H	1.27192900	-0.88094600	-1.55577800	C	-4.16961900	2.17700500	-1.82036000
C	-0.67528700	-4.24906800	2.02486600	C	-4.17292300	2.68375800	0.52058000
H	-1.47767900	-4.95771200	2.24946300	C	-5.33996700	2.91922300	-2.00216700
H	-0.37194000	-4.35046400	0.98332100	H	-3.73628600	1.68379500	-2.68892000
H	0.18032600	-4.52399500	2.65677700	C	-5.34625800	3.42835400	0.37386700
H	-0.18767200	-2.19175000	2.16795900	H	-3.72911600	2.59150200	1.50742900
H	-4.33866500	-2.79238300	0.14329600	C	-5.90638800	3.53276800	-0.89264500
C	-3.01408400	-4.37253100	-0.39047100	H	-5.81212300	3.01944800	-2.97485800
H	-2.47735500	-3.84871600	-1.18785600	H	-5.82429300	3.91898900	1.21657700
H	-2.32488800	-5.09222800	0.05702400	C	2.89509600	0.58745700	-0.69058900
H	-3.84000100	-4.93551900	-0.84286500	C	3.60789500	0.60753500	-1.90339800
C	-4.24637800	-4.11858300	1.82271500	C	3.45272400	-0.12081800	0.38415300
H	-5.06136100	-4.74775600	1.44308100	C	4.83945000	-0.04274800	-2.04083700
H	-3.54556700	-4.77082900	2.35077400	H	3.20893000	1.14260800	-2.76109200
H	-4.67650000	-3.42479100	2.55125000	C	4.68092200	-0.77873000	0.26668400
H	1.91274700	4.16604400	1.10508700	H	2.92411600	-0.19029500	1.32756500
C	1.38198800	0.14303000	3.24425500	C	5.35340900	-0.72408800	-0.94636600
H	0.59790500	-0.18639400	2.55847000	H	5.39117900	-0.02330200	-2.97594400
H	2.22276300	-0.54029400	3.11508800	H	5.10265200	-1.34376200	1.09180800
H	1.00812500	0.04036500	4.27101000	C	0.92789000	-2.65029000	-0.17978200
H	2.60684000	1.87491400	3.61549800	C	1.69517500	-3.18445600	-1.23075300
H	3.25967700	-0.29792400	1.17596800	C	1.42303200	-2.79435300	1.12625300
C	4.35689200	0.65789500	-0.37926400	C	2.91197900	-3.83277700	-0.99504100
H	4.99819500	-0.22326200	-0.49146000	H	1.34688100	-3.10521600	-2.25763800
H	3.57989800	0.59925300	-1.14600300	C	2.63089500	-3.44929100	1.38461000
H	4.96824500	1.54406000	-0.57046700	H	0.87708700	-2.38321200	1.96775700
C	3.63609900	3.94803300	-0.14316200	C	3.35624600	-3.95302100	0.31446800
H	3.65174700	5.03227300	-0.30577200	H	3.50835800	-4.23460700	-1.80846700
H	4.67370700	3.60699300	-0.07766900	H	3.01567700	-3.55145900	2.39500800
H	3.17765500	3.48264600	-1.01966200	F	-7.04802000	4.25540000	-1.05130600
C	3.64220900	4.14694500	2.37521100	F	4.54264400	-4.57117500	0.55514100
H	3.85532000	5.21494000	2.24093200	F	6.54669600	-1.36424900	-1.06819300
H	3.07480900	4.04154700	3.30390600	O	-1.93531300	0.89546000	1.00149300
H	4.59953700	3.63285400	2.49888000	H	-1.13746900	0.34315200	1.06026400
O	0.56261500	-3.18378300	-0.59258800	P	1.72956400	3.11578700	0.61933700
H	0.62875400	-3.50043300	-1.50536500	P	-2.09041600	-3.02295500	0.38776800
B	1.73371300	-2.35218000	-0.22933800	C	0.33753400	4.36861100	0.78511100
C	3.05912700	-2.75304700	-1.09284600	H	-0.12208300	4.33862700	-0.20826500
C	4.27558800	-3.04469600	-0.45525000	C	3.14685400	4.12006300	-0.07153100
C	3.06141200	-2.78440300	-2.49977200	H	3.14302400	5.05736200	0.49406700
C	5.44032000	-3.35063900	-1.16560300	C	-3.85789400	-2.45726200	0.07856600
H	4.31062300	-3.02095300	0.63091100	H	-3.77536500	-1.97549100	-0.90126100
C	4.20746500	-3.08227600	-3.24202500	C	-1.81706200	-3.35928400	2.20174000
H	2.14567100	-2.56481000	-3.05052200	H	-0.85099100	-3.87613600	2.19450100
C	5.38109500	-3.36020200	-2.55280600	C	-2.01643500	-4.71025800	-0.41717400
H	6.37768700	-3.57484600	-0.66475200	H	-2.93695900	-5.22005500	-0.11499100
H	4.20093900	-3.10107500	-4.32776700	C	-2.02496000	-4.54286200	-1.94299200
F	6.50623800	-3.65192300	-3.25977300	H	-2.86470600	-3.93164400	-2.29092700
O	1.93263200	-2.34309500	1.20443500	H	-1.10033000	-4.06418600	-2.28289400
H	1.86970600	-3.25438800	1.52251200	H	-2.10057800	-5.52474300	-2.42619100
9:				C	-0.83694200	-5.57930500	0.03383200
E: -2972.112589				H	-0.86342400	-5.79192300	1.10668300
G293: -2971.294425				H	-0.88577000	-6.54096200	-0.49252900
G243: -2971.273731				H	0.12319300	-5.11593000	-0.20221400
B	-2.17410200	1.22217600	-0.37826100	C	-4.30582100	-1.37831800	1.07394100
Pd	1.05473700	1.35707300	-0.68032200	H	-3.55783200	-0.59334500	1.20022800
Pd	-0.66867200	-1.53901800	-0.62173300	H	-5.22395200	-0.90965400	0.69865500
				H	-4.53552400	-1.81481100	2.05200500
				C	-4.90551400	-3.57529500	-0.01591500
				H	-5.88737400	-3.11761700	-0.19087900

H	-4.71704000	-4.26451500	-0.84354300
H	-4.97423500	-4.15747400	0.90816300
C	-1.64007100	-2.08223800	3.03421500
H	-2.58110100	-1.54368000	3.16318400
H	-1.26530000	-2.34879000	4.03032800
H	-0.92274900	-1.39434700	2.57735800
C	-2.85554800	-4.29994900	2.82609200
H	-2.53958200	-4.56922800	3.84172900
H	-3.83594700	-3.82020100	2.90078600
H	-2.97143500	-5.22789000	2.25759200
C	2.86282000	4.43654300	-1.54638200
H	2.87064000	3.52048000	-2.14662600
H	1.89015300	4.92130100	-1.68609900
H	3.63316500	5.11059600	-1.94060500
C	4.53069800	3.48481800	0.10585900
H	4.61216900	2.52849000	-0.41386000
H	5.28531200	4.16220700	-0.31369100
H	4.78155300	3.32762400	1.15912000
C	2.31125100	2.56302200	2.30275200
H	3.24309200	2.04117400	2.05763300
C	1.37302100	1.52804800	2.94071500
H	0.44404000	1.98049300	3.29518600
H	1.11101600	0.73524300	2.23245300
H	1.87167100	1.06549100	3.80171900
C	2.64425100	3.70617100	3.26870400
H	3.11544300	3.29729900	4.17138900
H	3.33917300	4.42955100	2.83049000
H	1.74330300	4.24320000	3.57980700
C	-0.73022800	3.91366000	1.78844500
H	-0.37897900	4.02919200	2.81932100
H	-1.61760700	4.54812300	1.67094700
H	-1.03932800	2.87943000	1.62692600
C	0.77162300	5.81314200	1.07030000
H	1.38337200	6.23670700	0.26895300
H	-0.12730800	6.43653300	1.15687300
H	1.32520600	5.90264700	2.01003200

9-THF:**E: -3204.697729****G293: -3203.764283****G243: -3203.741771**

B	-2.28250200	-0.34864000	0.11543200
Pd	-0.11930700	1.83635000	-0.53955700
Pd	0.73573200	-1.44266100	-0.23498600
O	-2.03453500	0.80814400	-0.86701500
O	-1.45288500	-1.52052800	-0.36157000
O	0.65423400	0.18056400	-1.59722300
H	-1.93841900	0.44433800	-1.76255000
H	-1.61465100	-1.64265600	-1.32215700
H	1.58803600	0.38059200	-1.77485600
C	-3.85508100	-0.73872800	0.11357700
C	-4.59827200	-0.83486600	-1.07658700
C	-4.53588600	-1.02579600	1.30860100
C	-5.94547500	-1.20751700	-1.08922300
H	-4.11918100	-0.61549000	-2.02750100
C	-5.88384600	-1.39684100	1.33117200
H	-3.99829100	-0.94752400	2.24886300
C	-6.56318700	-1.48331100	0.12364100
H	-6.51237300	-1.27972400	-2.01275200
H	-6.40447400	-1.61315500	2.25955100
C	1.74253800	2.50128100	-0.25594200
C	2.58614500	2.67032900	-1.36967600
C	2.31794200	2.63311700	1.01863000
C	3.94935500	2.94942000	-1.22454400
H	2.18404900	2.58785900	-2.37654100

C	3.67584200	2.92186000	1.18604900
H	1.71411100	2.49606900	1.90853000
C	4.46891200	3.06878900	0.05700000
H	4.59964000	3.06824100	-2.08590500
H	4.11847100	3.01240500	2.17364500
C	2.72140100	-1.26188000	-0.33377000
C	3.35976000	-1.60697600	-1.53922800
C	3.49495800	-0.64518500	0.66101500
C	4.72141400	-1.35954700	-1.74584700
H	2.79462800	-2.08181100	-2.33710000
C	4.85614400	-0.38555900	0.47351100
H	3.04015500	-0.34040800	1.59684500
C	5.44501600	-0.75190700	-0.72886300
H	5.21413000	-1.62925000	-2.67534400
H	5.44971500	0.10914300	1.23590900
F	-7.87566000	-1.84534100	0.12790000
F	6.76766800	-0.50068600	-0.91913100
F	5.79454400	3.32793500	0.21108500
O	-1.85785500	0.03938600	1.43557600
H	-0.90892300	0.24535600	1.40987900
P	-1.04624800	3.76561000	0.27617600
P	0.91173300	-3.18535900	1.23027000
C	-2.91368200	3.66378900	0.09324600
H	-3.02068000	3.05843600	-0.81250200
C	-0.57557100	5.25313400	-0.75522400
H	-1.30249600	6.03215500	-0.50288000
C	-0.77371700	-3.98422700	1.46588700
H	-1.20820100	-3.90444800	0.46373000
C	1.61958200	-2.64815700	2.87148200
H	2.66308300	-2.44085500	2.60843600
C	2.00737600	-4.60890000	0.70590300
H	1.73782800	-5.43610900	1.37058600
C	1.67230100	-5.01039200	-0.73620000
H	0.60015600	-5.17437000	-0.88692100
H	1.99505700	-4.23356800	-1.43530300
H	2.19399000	-5.93975600	-0.99634800
C	3.51137100	-4.36050600	0.87107200
H	3.78836300	-4.16548100	1.91119200
H	4.05362700	-5.25916600	0.55052400
H	3.85655500	-3.52433800	0.26023300
C	-1.66835000	-3.16706700	2.40693100
H	-1.66853900	-2.10424200	2.16100300
H	-2.69971900	-3.52999200	2.31819700
H	-1.36408300	-3.29392300	3.45150000
C	-0.76303100	-5.46336700	1.87469400
H	-1.80100500	-5.80299100	1.98250000
H	-0.28749300	-6.10605900	1.12856700
H	-0.26381000	-5.62429800	2.83538300
C	1.01937900	-1.32814300	3.37500000
H	-0.01569700	-1.44369600	3.70374100
H	1.60564900	-0.96391700	4.22815500
H	1.04143200	-0.55989300	2.59528200
C	1.60877700	-3.73643800	3.95181900
H	2.17299900	-3.39007800	4.82687800
H	0.59140800	-3.96463200	4.28281100
H	2.07157700	-4.66616100	3.60586300
C	-0.72609100	4.90402400	-2.24247300
H	0.00588200	4.14359000	-2.53589400
H	-1.72282300	4.51671100	-2.48001100
H	-0.55707200	5.79774400	-2.85575800
C	0.82211600	5.80869600	-0.45982000
H	1.60146500	5.06775600	-0.65092300
H	1.00720300	6.66987900	-1.11434000
H	0.92153100	6.15500000	0.57325300
C	-0.58531400	4.24415200	2.01919200
H	0.48306900	4.46534000	1.91744700
C	-0.71477000	3.08632700	3.01897800

H	-1.75701200	2.88062700	3.27158500
H	-0.28136700	2.16045100	2.63078800
H	-0.18898600	3.34725000	3.94596500
C	-1.28710600	5.50889600	2.52985100
H	-0.85102900	5.80534400	3.49213700
H	-1.17734400	6.35265300	1.84166600
H	-2.35536900	5.33538300	2.69019800
C	-3.56010200	2.87290100	1.23834100
H	-3.61714500	3.47648100	2.15090800
H	-4.58584300	2.60863400	0.95340100
H	-3.02403000	1.94717400	1.45503500
C	-3.63732200	4.99954500	-0.12407500
H	-3.32962400	5.50333300	-1.04466600
H	-4.71396600	4.80312600	-0.20545100
H	-3.49193300	5.69114600	0.71147500
C	-2.55492800	-2.96189200	-3.22366500
O	-1.98931400	-1.64629900	-3.07544900
C	-0.74674500	-1.68075400	-3.80709200
C	-0.13624900	-3.04971800	-3.47901000
C	-1.36321800	-3.92915400	-3.11291100
H	-3.31171100	-3.08362100	-2.44633800
H	-3.03892100	-3.03309400	-4.20753800
H	-0.96515300	-1.58035300	-4.87974400
H	-0.14973400	-0.83735200	-3.45733600
H	0.43851900	-3.45163200	-4.31856400
H	0.53361700	-2.95517300	-2.61875500
H	-1.48269200	-4.78527500	-3.78267400
H	-1.27190700	-4.31187700	-2.09173500

20:

E: -3479.897203

G293: -3478.96561

G243: -3478.942504

Pd	1.04248200	0.82987300	-0.23302600
O	-0.31470600	0.62510500	-1.86271200
Pd	-1.57423800	-0.59480300	-0.65685600
O	0.64420600	-1.40567400	-0.68462000
C	-3.04648800	0.67780100	-1.01625900
C	-2.93926100	1.95943400	-0.45147000
C	-4.07618900	0.42980000	-1.93289000
C	-3.85437000	2.96673500	-0.77013700
H	-2.13609000	2.18617200	0.24126400
C	-5.00298900	1.42711900	-2.25849700
H	-4.17163600	-0.54166000	-2.40621700
C	-4.87749400	2.67526000	-1.66372200
H	-3.77488800	3.95989300	-0.33861800
H	-5.80788100	1.24250500	-2.96346300
C	0.91201200	2.80664400	-0.33052200
C	0.24374500	3.59857100	0.61448700
C	1.36363700	3.42018500	-1.51198700
C	0.02982900	4.96426800	0.39630000
H	-0.12378400	3.16168400	1.53533500
C	1.16440100	4.78517600	-1.74286800
H	1.87912500	2.83453100	-2.26806300
C	0.49894900	5.53246700	-0.77975400
H	-0.49239700	5.57819500	1.12403300
H	1.51634700	5.26296200	-2.65216500
F	0.29911300	6.85861700	-0.99656600
F	-5.77709900	3.64442200	-1.97236800
P	2.42982400	0.86886700	1.58554700
P	-2.98299600	-1.84033100	0.66036100
C	3.21298100	2.50195500	2.04215200
C	1.50507800	0.35407800	3.12334400
C	3.70979900	-0.46635400	1.33456600
C	0.51624500	1.42155100	3.60511600

H	-0.27299200	1.58374500	2.86488100
H	0.03493300	1.07832800	4.52909800
H	0.99466700	2.38202400	3.81872000
C	4.39179600	-1.00519700	2.59789800
H	3.67558400	-1.39101000	3.32875400
H	5.04593300	-1.83818300	2.31096300
H	5.01290800	-0.24974000	3.08844500
C	-3.87263600	-0.89947400	2.01566900
H	-4.23980600	-1.67115800	2.69961600
C	-2.02261200	-3.16876200	1.58796200
C	-4.35929900	-2.62092900	-0.32826300
C	-2.87554500	-0.01385800	2.77223500
H	-2.04139500	-0.58951400	3.18135100
H	-2.46208000	0.75575100	2.11361700
H	-3.38010300	0.48687400	3.60780600
C	-5.09167700	-0.09032100	1.55464700
H	-4.81964900	0.71076200	0.86616100
H	-5.85176700	-0.71445800	1.07663200
H	-5.55468700	0.36926600	2.43704300
C	-2.62893500	-3.61594300	2.92509500
H	-1.98284900	-4.38911200	3.35913000
H	-2.69545000	-2.80202400	3.65168300
H	-3.62528900	-4.05070600	2.79959600
H	-0.75715500	1.46639100	-2.06108300
H	0.57184300	-1.20433000	-1.63608400
C	-1.71979400	-4.38559900	0.70173400
H	-2.62420800	-4.96883400	0.50713100
H	-1.25481400	-4.11187900	-0.24925700
H	-1.02383500	-5.04830600	1.23390200
H	-1.07389400	-2.66685800	1.80459800
H	-4.95210700	-1.74418700	-0.61039000
C	-3.86522700	-3.26302900	-1.63244500
H	-3.16308200	-2.60981800	-2.16166800
H	-3.36321600	-4.21701900	-1.45539000
H	-4.72156800	-3.45290600	-2.29129600
C	-5.26767100	-3.56364000	0.47174000
H	-6.12475500	-3.85440200	-0.14848700
H	-4.74516600	-4.47939800	0.76270600
H	-5.66051500	-3.09289400	1.37837000
H	2.33216800	3.13945400	2.17560200
C	0.77525500	-0.96853200	2.86847000
H	-0.00227900	-0.82244400	2.11295400
H	1.42931300	-1.76090700	2.49955500
H	0.29580000	-1.31021700	3.79465100
H	2.26236900	0.20428300	3.90101000
H	3.10670500	-1.27736800	0.91424400
C	4.74584700	-0.06271500	0.27820200
H	5.27758400	-0.95600300	-0.06273600
H	4.28319900	0.40285700	-0.59702400
H	5.48487200	0.63060200	0.69044000
C	4.05210800	3.12720800	0.91895900
H	4.19280900	4.19420100	1.13050000
H	5.04247800	2.66992400	0.85538300
H	3.56900200	3.04142300	-0.05623600
C	3.99785100	2.48595100	3.36055100
H	4.28528800	3.51282700	3.61899600
H	3.41717300	2.08566500	4.19649900
H	4.91798600	1.90070700	3.27091800
B	1.38814200	-2.77841100	-0.69083100
C	2.86276500	-2.59944400	-1.35661900
C	3.94128100	-3.38926300	-0.92177600
C	3.11053800	-1.74458000	-2.44605100
C	5.20123800	-3.33971600	-1.52657600
H	3.78973300	-4.05758200	-0.07858300
C	4.35839100	-1.66523700	-3.07008900
H	2.31548500	-1.10934800	-2.83321200
C	5.38412500	-2.47119200	-2.59419900

H	6.02813300	-3.95483900	-1.18356900
H	4.53920700	-0.99780300	-3.90753300
O	0.49663000	-3.57421800	-1.55375600
H	0.96312100	-4.38279500	-1.81291100
O	1.52250000	-3.26379300	0.66208000
H	0.65757800	-3.58808500	0.94750500
F	6.60471000	-2.40729200	-3.19250800

21:**E: -3479.896098****G293: -3478.966687****G243: -3478.943326**

Pd	-2.58525000	-0.50709800	-0.28551300
Pd	2.60270300	0.64261900	-0.02781300
B	-0.45147500	1.77955100	-0.13215300
B	0.49640600	-1.78029000	-0.75715200
O	-0.97485700	-1.97175800	-0.41182400
O	-1.14128800	0.88492900	-1.08528900
O	1.12265200	-0.95679500	0.30825600
O	0.97562700	1.90489300	-0.64615800
H	-1.08214100	-2.74453900	0.15846500
H	-0.47144800	0.30572700	-1.53325100
H	0.44022300	-0.36104300	0.71225800
H	1.26641300	2.82683900	-0.70343700
C	3.73048800	2.25914800	-0.28032800
C	4.05933200	2.67460300	-1.58117400
C	4.06581600	3.10408100	0.79024500
C	4.71470000	3.88895900	-1.81306600
H	3.80660900	2.04781600	-2.43237100
C	4.71753200	4.32400800	0.57742900
H	3.82590400	2.81395900	1.80919500
C	5.03365800	4.68976200	-0.72442300
H	4.97420700	4.21164300	-2.81685100
H	4.97714400	4.98110000	1.40206700
C	-3.91054500	0.97635900	-0.21350800
C	-4.79634700	1.25752600	-1.26160700
C	-3.84156400	1.88021400	0.85856200
C	-5.59729600	2.40692000	-1.24697500
H	-4.86995700	0.58908000	-2.11389300
C	-4.63694800	3.02781400	0.89527900
H	-3.14101000	1.70564900	1.66746600
C	-5.50207500	3.26872800	-0.16407800
H	-6.27934000	2.63353100	-2.06109700
H	-4.57289900	3.73682000	1.71442500
C	1.15089400	-3.26184000	-0.81684700
C	1.61023900	-3.84673400	-2.00640800
C	1.22071200	-4.05184300	0.34624700
C	2.13477600	-5.14227300	-2.04811600
H	1.57903000	-3.27296800	-2.92910900
C	1.73679800	-5.34946400	0.34029600
H	0.88175200	-3.63700300	1.29282300
C	2.19097800	-5.86821900	-0.86625000
H	2.49677600	-5.58531800	-2.97094100
H	1.79482200	-5.95002000	1.24304400
C	-1.12735300	3.24444000	-0.08579000
C	-1.07228200	4.06179700	1.05502300
C	-1.80009600	3.75980400	-1.20671000
C	-1.67358700	5.32258100	1.09934300
H	-0.57015400	3.70463500	1.95254800
C	-2.41543600	5.01263200	-1.19464900
H	-1.87331900	3.14645100	-2.09993600
C	-2.34245700	5.76972900	-0.03232300
H	-1.63811000	5.94619600	1.98753700
H	-2.95304200	5.39750600	-2.05588300
P	4.39327900	-0.58190300	0.68291200

P	-4.21168000	-1.96464600	0.39108900
C	4.18198200	-1.06704900	2.47301400
H	5.12472400	-1.53437600	2.77631300
C	6.06774900	0.26044200	0.65221300
H	5.83539100	1.27239300	0.99666700
C	4.44785100	-2.17595700	-0.27564600
H	3.49696700	-2.63823500	0.00625200
C	-5.54544200	-2.13281100	-0.90070800
H	-6.03378600	-1.15373100	-0.83643900
C	-5.11403200	-1.57322600	1.97879200
H	-5.59672800	-2.51177300	2.26928000
C	-3.44133900	-3.64800200	0.74438300
H	-2.52979600	-3.38614100	1.29806400
O	0.53796800	-1.02487800	-2.01589400
H	0.06355500	-1.52015500	-2.70175700
O	-0.41941500	1.08300200	1.17886100
H	0.12304500	1.58380900	1.80788500
C	3.05358100	-2.08006500	2.68717000
H	2.10837400	-1.71334300	2.28050000
H	3.27233600	-3.03974900	2.21045600
H	2.93238200	-2.26254100	3.76269500
C	3.96111500	0.19561900	3.31723500
H	4.75878000	0.93375500	3.18323800
H	3.01064900	0.67353300	3.05196200
H	3.92455900	-0.06912200	4.38099200
C	6.63220100	0.37544800	-0.76974300
H	7.01677700	-0.58672800	-1.12197100
H	5.88879400	0.73573600	-1.48420400
H	7.46698200	1.08658700	-0.76893400
C	7.11972800	-0.32614800	1.60461300
H	7.34035800	-1.37498500	1.38771000
H	8.05255900	0.23927700	1.48623200
H	6.82366100	-0.24695400	2.65409500
C	4.39139500	-1.94195800	-1.79179800
H	3.54650000	-1.30088300	-2.06189000
H	5.30785400	-1.48583700	-2.17382300
H	4.25901100	-2.90418800	-2.29753600
C	5.58172700	-3.13065500	0.11404100
H	5.41247500	-4.10232300	-0.36628000
H	6.55525400	-2.75907400	-0.22135700
H	5.63230800	-3.29975700	1.19457100
C	-4.09038100	-1.19572400	3.05799100
H	-3.31680000	-1.96215100	3.17986900
H	-3.59193300	-0.25410900	2.80840400
H	-4.59439300	-1.07104100	4.02408700
C	-6.21904800	-0.51829500	1.84973900
H	-5.82903900	0.44969700	1.53258900
H	-7.00022200	-0.82421800	1.14761900
H	-6.69315100	-0.38628300	2.83052200
C	-3.03883500	-4.37840100	-0.54719600
H	-3.91695900	-4.81388700	-1.03330200
H	-2.53657200	-3.72517700	-1.26417900
H	-2.35354600	-5.19867600	-0.30189200
C	-4.24435400	-4.58545700	1.65847400
H	-5.23028300	-4.82045500	1.24834800
H	-3.69429800	-5.52928600	1.75981400
H	-4.37582600	-4.17681000	2.66377200
C	-4.98087100	-2.26185900	-2.32297900
H	-4.58896700	-3.26393900	-2.51475100
H	-5.77978400	-2.07160700	-3.05001300
H	-4.17370700	-1.54425700	-2.50345400
C	-6.59138900	-3.21455500	-0.60757900
H	-7.41926100	-3.12367200	-1.32169900
H	-6.16837900	-4.21758300	-0.71869500
H	-7.01074100	-3.12834200	0.39957600
F	-2.94486200	6.98839400	-0.00095400
F	2.70302500	-7.12679900	-0.88925200

F -6.27418800 4.38850600 -0.14224600
 F 5.67191700 5.87021800 -0.93972600

21-THF:

E: -3712.477996

G293: -3711.435205

G243: -3711.409856

Pd -2.80527000 -0.34685600 -0.16152400
 Pd 2.54861700 -0.19883200 0.18803800
 B -0.27630700 1.46920100 0.37660600
 B 0.01649400 -2.15985400 -0.47069500
 O -1.45544500 -2.04819800 -0.09579800
 O -1.06269500 0.79863700 -0.69372900
 O 0.81885100 -1.51305200 0.59660100
 O 1.16362600 1.42424900 -0.03247700
 H -1.70391800 -2.75359900 0.51682400
 H -0.49283000 0.12655600 -1.14430700
 H 0.25539000 -0.82719000 1.04590800
 H 1.54689300 2.29276200 -0.28584400
 C 3.95218900 1.15545900 -0.17806500
 C 4.26394000 1.47695200 -1.50715000
 C 4.50050400 1.94267700 0.84492900
 C 5.07950700 2.56948700 -1.81685700
 H 3.85131800 0.88665800 -2.32112000
 C 5.31384200 3.04335800 0.55487800
 H 4.28210300 1.71608500 1.88483800
 C 5.57643300 3.33866400 -0.77503500
 H 5.31149300 2.83371300 -2.84421100
 H 5.72406700 3.67118500 1.34030900
 C -3.87363300 1.33013400 -0.19626300
 C -4.50443600 1.81134100 -1.35057300
 C -3.86007500 2.14957300 0.94377300
 C -5.10410700 3.07757200 -1.37616700
 H -4.53005700 1.21003100 -2.25443400
 C -4.45665300 3.41244100 0.94044300
 H -3.36172800 1.81407200 1.84674200
 C -5.06747200 3.85310700 -0.22647200
 H -5.58701900 3.45909400 -2.27097900
 H -4.43241000 4.05429600 1.81510200
 C 0.32786300 -3.74731000 -0.58337800
 C 0.52617700 -4.39910300 -1.81016500
 C 0.31829200 -4.55556000 0.56868100
 C 0.72739500 -5.77975100 -1.89972600
 H 0.54421000 -3.81581500 -2.72740800
 C 0.51467500 -5.93745700 0.51582800
 H 0.17190100 -4.09163300 1.54122900
 C 0.72139800 -6.52303500 -0.72718500
 H 0.88898000 -6.27579800 -2.85205200
 H 0.51430900 -6.55349000 1.41003700
 C -0.76518600 3.00200700 0.54950700
 C -0.82152700 3.64338900 1.79578100
 C -1.15038100 3.75803300 -0.57096200
 C -1.25519100 4.96582000 1.93875300
 H -0.54549700 3.09626500 2.69500200
 C -1.58978300 5.07861000 -0.46593800
 H -1.13403900 3.28854600 -1.55024600
 C -1.63594000 5.65716900 0.79724000
 H -1.30828600 5.45245700 2.90812600
 H -1.90610100 5.65072000 -1.33294200
 P 4.13028200 -1.78465700 0.63040100
 P -4.72564900 -1.55489100 0.11984700
 C 4.01907300 -2.28020200 2.42798200
 H 4.87647300 -2.93297900 2.62257800
 C 5.92888300 -1.28628100 0.42613800
 H 5.93494500 -0.25289500 0.78494800

C 3.77649700 -3.33324100 -0.33895600
 H 2.78437400 -3.60579500 0.03336600
 C -5.78668900 -1.45023100 -1.41016400
 H -6.12758300 -0.40952300 -1.36661800
 C -5.85879300 -1.09620700 1.53125300
 H -6.53218200 -1.95187600 1.64553500
 C -4.29512500 -3.35208600 0.48677400
 H -3.47987800 -3.25974300 1.21635700
 O 0.19108300 -1.39631800 -1.71306400
 H -0.39725400 -1.75160100 -2.39722300
 O -0.41888700 0.64859600 1.61130500
 H 0.19417700 0.98849600 2.28173700
 C 2.74019900 -3.05882200 2.75070400
 H 1.85005800 -2.50217600 2.44823700
 H 2.71543600 -4.02858900 2.24539900
 H 2.69397200 -3.24553500 3.83140000
 C 4.13980800 -1.02725800 3.30624700
 H 5.04379000 -0.44909800 3.08816900
 H 3.27535400 -0.36988100 3.15597800
 H 4.17162700 -1.31470100 4.36436600
 C 6.36361800 -1.26529800 -1.04521600
 H 6.50954000 -2.27912300 -1.43061900
 H 5.64344400 -0.75077200 -1.68461500
 H 7.32118400 -0.73726200 -1.12947100
 C 6.93575900 -2.08087200 1.27044300
 H 6.92681000 -3.14883400 1.03467900
 H 7.94437300 -1.70434400 1.05812900
 H 6.76595700 -1.96409500 2.34413100
 C 3.61965900 -3.05519900 -1.84034100
 H 2.89030100 -2.25954000 -2.02009700
 H 4.56521400 -2.77472400 -2.31019300
 H 3.25556800 -3.96192400 -2.33527300
 C 4.72877000 -4.50310400 -0.06812200
 H 4.32639200 -5.40902200 -0.53839600
 H 5.72240700 -4.32219900 -0.49040500
 H 4.84350300 -4.70844500 1.00120800
 C -5.02758600 -0.95315800 2.81314900
 H -4.43996900 -1.85343100 3.02518000
 H -4.33401100 -0.11004400 2.73515300
 H -5.68856200 -0.77477400 3.67001000
 C -6.73375400 0.13765200 1.28083500
 H -6.13936000 1.04020000 1.13296100
 H -7.38915800 0.00884600 0.41436200
 H -7.37556200 0.29546800 2.15680400
 C -3.75828500 -4.08454200 -0.75299100
 H -4.57506700 -4.34547300 -1.43276600
 H -3.02049100 -3.49539600 -1.30038700
 H -3.27508700 -5.01809700 -0.44042800
 C -5.39305100 -4.18402400 1.16562600
 H -6.30394100 -4.23694700 0.56316800
 H -5.02331000 -5.20832100 1.29872700
 H -5.65517100 -3.80137600 2.15543800
 C -4.97492500 -1.60209800 -2.70482800
 H -4.69036800 -2.64157000 -2.88687700
 H -5.58130300 -1.26830800 -3.55577600
 H -4.05974800 -1.00106400 -2.67815900
 C -7.01930400 -2.36183200 -1.40456600
 H -7.66505500 -2.10649600 -2.25399000
 H -6.73835400 -3.41441600 -1.50865700
 H -7.61352400 -2.25404100 -0.49175500
 F -2.07483300 6.93973200 0.91869200
 F 0.92057900 -7.86586800 -0.79692400
 F -5.64329100 5.08579500 -0.24327100
 F 6.32583700 4.43960600 -1.06895200
 C 2.26446900 4.94216200 0.26782100
 O 2.19193500 3.88181000 -0.68934900
 C 2.13800000 4.50731400 -1.97256700

C	3.11646200	5.69129500	-1.88345300
C	3.20756500	5.98176600	-0.36076100
H	1.26265600	5.36040800	0.42981100
H	2.62881800	4.51425100	1.20377600
H	2.40996500	3.75542000	-2.71607600
H	1.11322500	4.85389100	-2.16920400
H	4.09863500	5.41449100	-2.27482800
H	2.75343000	6.55049000	-2.45479900
H	4.23300700	5.84004200	-0.01003700
H	2.90026500	7.00059700	-0.10758700

PPh₃ COMPOUNDS

3-PPh₃:

E: -2608.347544

G293: -2607.760616

G243: -2607.744023

Pd	-0.00895900	-0.45870900	-0.10052500
P	2.31576800	-0.45591700	-0.01306400
P	-2.34217100	-0.39926800	-0.04336100
C	3.04911500	-0.38374100	-1.68300200
C	2.24650900	-0.75844300	-2.77103900
C	4.37708600	0.01108500	-1.90646300
C	2.76715500	-0.74222500	-4.06566400
H	1.21706800	-1.05841000	-2.59416700
C	4.89276200	0.02805100	-3.20248000
H	5.00310700	0.31083300	-1.07204700
C	4.08925200	-0.34792800	-4.28244700
H	2.13888900	-1.03214700	-4.90308900
H	5.92095100	0.33654800	-3.36892500
H	4.49280600	-0.32991000	-5.29090600
C	2.96266700	-1.98957000	0.75377700
C	2.29514400	-2.48535800	1.88695300
C	4.07901100	-2.67649500	0.25911700
C	2.75137500	-3.63861700	2.52518100
H	1.41899200	-1.96518900	2.26347900
C	4.52585600	-3.83636600	0.89444800
H	4.59654700	-2.31296900	-0.62218200
C	3.86660600	-4.31704300	2.02784800
H	2.22933700	-4.01167200	3.40163200
H	5.38972700	-4.36487400	0.50132400
H	4.21643200	-5.22102300	2.51819100
C	3.12354600	0.89881000	0.91924200
C	3.48968000	0.73271400	2.26146400
C	3.26305200	2.16213000	0.32264000
C	3.98102100	1.81385200	2.99642100
H	3.39487000	-0.23714600	2.73831900
C	3.75514300	3.23760300	1.05879900
H	2.97423600	2.31025100	-0.71091000
C	4.11236500	3.06817800	2.39913100
H	4.26314900	1.67107900	4.03587300
H	3.85124600	4.21061500	0.58555700
H	4.49102600	3.90915700	2.97319300
C	-3.12704400	-0.94901200	-1.60244200
C	-2.46418700	-1.93756900	-2.34895800
C	-4.35370400	-0.44066000	-2.05322300
C	-3.02972700	-2.40569600	-3.53549700
H	-1.52257200	-2.33769600	-1.97636700
C	-4.90947700	-0.91133100	-3.24439800
H	-4.87105800	0.32329200	-1.48226300
C	-4.24833000	-1.89195500	-3.98731800
H	-2.51543600	-3.17123700	-4.11046900
H	-5.85848800	-0.51118800	-3.59047500
H	-4.68208600	-2.25479000	-4.91514900
C	-3.10838500	1.21684000	0.33786100

C	-3.63809200	1.49431100	1.60392800
C	-3.02880400	2.24744300	-0.61289100
C	-4.07440700	2.78414600	1.91731200
H	-3.70534400	0.70948300	2.34990400
C	-3.46450900	3.53163600	-0.29793100
H	-2.61035500	2.04758700	-1.59340300
C	-3.98448900	3.80500600	0.97117500
H	-4.48260300	2.98754100	2.90348600
H	-3.38782900	4.32210600	-1.03897300
H	-4.31617000	4.80948300	1.21860700
C	-2.99685000	-1.51643500	1.24826700
C	-4.28701200	-2.05747200	1.17517800
C	-2.19156800	-1.79538000	2.36129600
C	-4.76618500	-2.86565200	2.20706800
H	-4.91521200	-1.85142900	0.31393100
C	-2.67589800	-2.59636000	3.39563500
H	-1.18395400	-1.39225400	2.40155900
C	-3.96318000	-3.13382400	3.31855700
H	-5.76588400	-3.28603900	2.14225500
H	-2.04568900	-2.80970200	4.25459500
H	-4.33801000	-3.76446300	4.11993600
C	0.06812700	1.56415900	-0.03126900
C	-0.06785400	2.28525900	1.16518300
C	0.25008800	2.29712000	-1.21500900
C	-0.02842800	3.68174000	1.19121400
H	-0.21343100	1.75489900	2.10324500
C	0.29102100	3.69660600	-1.21645300
H	0.36498100	1.77574600	-2.16279300
C	0.15009700	4.36155500	-0.00672600
H	-0.13877200	4.23875300	2.11680800
H	0.43048400	4.26322400	-2.13263200
O	-0.15829900	-2.52300400	-0.34292300
H	0.67246100	-2.91365200	-0.03342200
F	0.18776200	5.72343700	0.00702800

3-PPh₃-cis:

E: -2608.346557

G293: -2607.758365

G243: -2607.741878

Pd	0.34662000	-1.18472600	0.06048600
P	1.19282600	0.94472500	-0.04425600
C	0.96113700	1.77426000	-1.65858600
C	0.16070200	1.16192800	-2.63088300
C	1.59996100	2.98848200	-1.96217300
C	-0.03126900	1.76801000	-3.87348600
H	-0.30474200	0.20727300	-2.41277700
C	1.40468000	3.59402000	-3.20211400
H	2.26284300	3.44979300	-1.23701900
C	0.58391900	2.98734200	-4.15783800
H	-0.65991900	1.28554000	-4.61631800
H	1.90006500	4.53444100	-3.42623900
H	0.43529600	3.46006700	-5.12460300
C	2.98950100	1.15658200	0.25258500
C	3.48266500	1.57318000	1.49399300
C	3.89134900	0.78139000	-0.75548000
C	4.85960300	1.60182800	1.72942200
H	2.79799300	1.86681100	2.28257100
C	5.26256200	0.80675800	-0.51654200
H	3.51984500	0.44973000	-1.71944300
C	5.75075900	1.21380800	0.72934800
H	5.23188100	1.92567000	2.69742700
H	5.95069700	0.50138600	-1.29952400
H	6.82075900	1.22684200	0.91663000
C	0.43119600	2.00397300	1.24452200
C	0.26869000	3.38965800	1.12137000

C	-0.00905100	1.36214500	2.41201600	C	-1.62513200	0.80610500	2.61177600
C	-0.34068300	4.11674800	2.14433200	C	-1.88015400	3.21260900	2.44361200
H	0.58663200	3.90154500	0.22061700	C	-2.01484600	0.86237700	3.95041300
C	-0.62068000	2.08946700	3.43334700	H	-1.40575400	-0.14429300	2.13492100
H	0.10647700	0.28718600	2.50548100	C	-2.26557300	3.26197700	3.78447900
C	-0.79213700	3.46904800	3.29773800	H	-1.83451200	4.12782900	1.86270400
H	-0.47398400	5.18930200	2.03448900	C	-2.32968300	2.08919400	4.54039800
H	-0.97578900	1.57496400	4.32148100	H	-2.07110400	-0.05364300	4.53216300
H	-1.27799400	4.03751600	4.08567800	H	-2.51597400	4.21740500	4.23693800
C	2.25202400	-1.89048600	0.08593500	H	-2.62750300	2.13139700	5.58437300
C	3.06413400	-1.83904700	1.22802400	C	-2.63064700	1.68116500	-0.82758500
C	2.78756300	-2.46342100	-1.07626800	C	-2.57359300	1.34511200	-2.18931000
C	4.37681200	-2.32210200	1.21537200	C	-3.87757400	1.83002700	-0.20790600
H	2.69118600	-1.38780800	2.14393300	C	-3.74809900	1.16875200	-2.91902000
C	4.10242700	-2.94262800	-1.11692000	H	-1.61082400	1.20165400	-2.66829700
H	2.18010400	-2.53791000	-1.97508000	C	-5.05152600	1.63781200	-0.93821200
C	4.87356400	-2.85554300	0.03385100	H	-3.93566700	2.07708300	0.84645300
H	5.01134500	-2.27144600	2.09509600	C	-4.98952800	1.30504300	-2.29176100
H	4.52433700	-3.37647100	-2.01897700	H	-3.69363000	0.90678400	-3.97207700
F	6.15849400	-3.30798100	0.00330400	H	-6.01346800	1.73523500	-0.44358600
P	-2.00283300	-0.60703800	0.01883000	H	-5.90432600	1.14461100	-2.85496600
O	-0.18089400	-3.15787300	0.26638400	C	-0.42166800	3.51055300	-0.34908900
H	-1.08067800	-3.24943300	-0.08292600	C	-0.82829800	4.17358500	-1.51383100
C	-2.89905100	-1.86357900	-0.97509100	C	0.59245600	4.07727600	0.44090100
C	-2.27841800	-2.35279000	-2.13662700	C	-0.22014700	5.37358900	-1.89045600
C	-4.18024800	-2.31902600	-0.63668400	H	-1.61722900	3.75928100	-2.13168400
C	-2.93799800	-3.27097600	-2.95441200	C	1.19674300	5.27331500	0.06267600
H	-1.27670800	-2.01704300	-2.39122000	H	0.91637700	3.57758200	1.34628700
C	-4.83288200	-3.24513300	-1.45129000	C	0.79632800	5.92254700	-1.10882500
H	-4.66635000	-1.95475700	0.26256700	H	-0.54531000	5.87725600	-2.79655700
C	-4.21547500	-3.71937400	-2.61129200	H	1.98640600	5.69375200	0.67867400
H	-2.44980800	-3.64281700	-3.85070100	H	1.27352300	6.85179100	-1.40707600
H	-5.82396000	-3.59680000	-1.17869300	C	2.77263600	-1.57697400	1.66508100
H	-4.72582700	-4.44137200	-3.24241900	C	2.03043100	-1.04978200	2.73406400
C	-2.72711500	-0.71652500	1.69731200	C	4.09689300	-1.97922100	1.87974400
C	-3.89579300	-0.03814600	2.07213800	C	2.60609600	-0.92403500	3.99734100
C	-2.06188700	-1.51634200	2.64059100	H	1.00715100	-0.72443000	2.56649800
C	-4.38035600	-0.14274500	3.37688400	C	4.67354400	-1.84473900	3.14463000
H	-4.42226100	0.57975800	1.35263500	H	4.67927900	-2.39418400	1.06385800
C	-2.55259000	-1.62171800	3.94214800	C	3.93142600	-1.31716200	4.20330600
H	-1.16595500	-2.05436800	2.34223800	H	2.02378700	-0.51036000	4.81591600
C	-3.70773100	-0.92944900	4.31473900	H	5.70314200	-2.15390600	3.30122500
H	-5.28279200	0.39206600	3.65957500	H	4.38412600	-1.21118400	5.18513300
H	-2.02915300	-2.24033000	4.66586900	C	3.26442600	-1.86422700	-1.19755600
H	-4.08401200	-1.00481700	5.33114000	C	3.26182200	-2.87674700	-2.16763700
C	-2.64578400	0.97220400	-0.66751100	C	4.27840700	-0.89106800	-1.23037200
C	-2.59954800	2.14916500	0.09577800	C	4.24965000	-2.91284400	-3.15386900
C	-3.09156500	1.04356900	-1.99587000	H	2.49459200	-3.64291700	-2.15510400
C	-2.97562400	3.36969800	-0.46405100	C	5.26665300	-0.93656800	-2.21215800
H	-2.28080600	2.11505600	1.12947200	H	4.30093300	-0.10241500	-0.48837400
C	-3.46516500	2.26637000	-2.55331700	C	5.25378800	-1.94426300	-3.17976600
H	-3.14297500	0.14639400	-2.60294700	H	4.23404900	-3.70482100	-3.89748900
C	-3.40302600	3.43444100	-1.79160100	H	6.04448400	-0.17814700	-2.22103800
H	-2.92989900	4.26990600	0.14191400	H	6.02297600	-1.97509600	-3.94641400
H	-3.80418700	2.30363500	-3.58476300	C	1.20534800	-3.42872200	0.10919100
H	-3.69044500	4.38712100	-2.22740000	C	1.59181000	-4.36801700	1.07514600
6-PPh₃:				C	0.24455800	-3.78168700	-0.85060500
E: -3039.655957				C	1.02621100	-5.64462300	1.07819600
G293: -3038.981274				H	2.33077100	-4.10873800	1.82549600
G243: -3038.962556				C	-0.31017700	-5.06137300	-0.84866800
Pd	0.38393900	0.00921600	-0.13340100	H	-0.08153300	-3.05478300	-1.58563800
P	-1.05856500	1.85168100	0.09248200	C	0.07619400	-5.99438700	0.11682400
P	1.92496300	-1.74534600	0.05224400	H	1.33056200	-6.36448500	1.83292500
C	-1.55044700	1.98521100	1.85127400	H	-1.05597900	-5.32295900	-1.59432600
				H	-0.36433900	-6.98755900	0.12270000
				C	1.94851000	1.25224500	-0.39116900
				C	2.21978300	1.74331000	-1.67883800

C	2.77614000	1.67819100	0.65831900
C	3.27682300	2.62480800	-1.92035100
H	1.59679600	1.43982200	-2.51681000
C	3.84298400	2.55795900	0.44036400
H	2.60278000	1.32155800	1.66883300
C	4.07137100	3.01515200	-0.84984100
H	3.48479300	3.00658300	-2.91541300
H	4.48405800	2.88702100	1.25298200
O	-1.31945500	-1.18760900	0.17941800
F	5.10377600	3.87341900	-1.07345200
B	-2.11190300	-1.49604300	-0.83617500
C	-3.65573900	-1.79235700	-0.59255300
C	-4.52909800	-2.27778100	-1.58047400
C	-4.21382100	-1.49345600	0.66356100
C	-5.89513500	-2.44955700	-1.34680800
H	-4.15198700	-2.53780600	-2.56804900
C	-5.57318600	-1.65292000	0.92913500
H	-3.56193000	-1.10986500	1.44195800
C	-6.39021500	-2.12622000	-0.09055000
H	-6.56731800	-2.82232800	-2.11331400
H	-6.00286000	-1.41285900	1.89691000
F	-7.71767300	-2.27966300	0.14969900
O	-1.61180400	-1.54630900	-2.15162400
H	-2.32233100	-1.64616200	-2.80223400

6-PPh₃-cis:**E: -3039.653785****G293: -3038.978928****G243: -3038.960214**

Pd	-0.09639100	0.65450600	-0.14617100
P	-2.31003300	0.16876800	0.16094100
C	-3.12521500	-0.50577000	-1.32765300
C	-2.33198100	-0.85459100	-2.42802900
C	-4.51941500	-0.65957600	-1.40838300
C	-2.91619000	-1.37907000	-3.58181100
H	-1.25861500	-0.70825600	-2.37489300
C	-5.10046500	-1.18600900	-2.56061800
H	-5.14973100	-0.35301300	-0.57977300
C	-4.29922200	-1.55085100	-3.64693900
H	-2.29005700	-1.65170000	-4.42630000
H	-6.17885100	-1.30475900	-2.61408500
H	-4.75527000	-1.95898000	-4.54446700
C	-3.40446000	1.55375400	0.65749600
C	-3.65132400	1.82032300	2.00982900
C	-3.90444000	2.42943800	-0.31818600
C	-4.38062900	2.95142800	2.38205300
H	-3.27182200	1.15207400	2.77581800
C	-4.62840500	3.55881000	0.05687500
H	-3.71352800	2.23863300	-1.36838900
C	-4.86638200	3.82465300	1.40842200
H	-4.56640600	3.14791300	3.43433500
H	-5.00118600	4.23547200	-0.70670300
H	-5.42728600	4.70850800	1.69877700
C	-2.53375500	-1.04078400	1.51937000
C	-3.58645500	-1.96338100	1.57113200
C	-1.58232300	-1.02425000	2.54982500
C	-3.67350600	-2.86565500	2.63141000
H	-4.32070100	-2.00321300	0.77496700
C	-1.66777700	-1.93000600	3.60741200
H	-0.76165300	-0.31609800	2.50578000
C	-2.71253900	-2.85596400	3.64664400
H	-4.48622000	-3.58608100	2.65753200
H	-0.90928200	-1.92146800	4.38460400
H	-2.77647300	-3.57040300	4.46247100
C	-0.64175500	2.59698000	-0.35303200

C	-0.81930900	3.45693500	0.73909700
C	-0.84608100	3.10937300	-1.64126700
C	-1.20814200	4.78753500	0.56036600
H	-0.66657700	3.09035900	1.74903700
C	-1.23764400	4.43907200	-1.84402500
H	-0.71298800	2.47070500	-2.51169800
C	-1.41856400	5.24956500	-0.73283400
H	-1.35864200	5.45531400	1.40335300
H	-1.40511400	4.83900700	-2.83983400
F	-1.81542800	6.53990000	-0.91461500
P	0.79846900	-1.61113900	-0.14854000
O	1.86680700	1.25173500	-0.40404800
C	2.22419500	-1.66123000	-1.30269300
C	2.13069300	-0.93590500	-2.50049500
C	3.37940800	-2.40711200	-1.04279700
C	3.16486700	-0.97925100	-3.43415500
H	1.25635300	-0.32043300	-2.68837500
C	4.42245000	-2.43618900	-1.97173000
H	3.47350100	-2.96050700	-0.11450700
C	4.31526500	-1.72908900	-3.17026200
H	3.08236300	-0.41221100	-4.35713800
H	5.31823700	-3.01154900	-1.75533200
H	5.12701700	-1.75288800	-3.89196100
C	1.46729400	-2.19656700	1.45316000
C	1.63932700	-3.55796600	1.74566500
C	1.82663700	-1.23788800	2.41221600
C	2.14785100	-3.95295800	2.98354400
H	1.36858300	-4.31067700	1.01294500
C	2.34098100	-1.63690800	3.64654900
H	1.70175800	-0.18104000	2.19960700
C	2.49707600	-2.99401800	3.93743500
H	2.27117400	-5.01012600	3.20154900
H	2.61369000	-0.88527000	4.38235900
H	2.88956300	-3.30391500	4.90193600
C	-0.24077500	-3.01139700	-0.73837100
C	-1.14956900	-3.63184500	0.13307500
C	-0.21930800	-3.40562200	-2.08450600
C	-2.02766900	-4.60779800	-0.33698100
H	-1.16649100	-3.36458300	1.18169200
C	-1.09853300	-4.38271800	-2.55190000
H	0.48086400	-2.94808500	-2.77479800
C	-2.01087100	-4.98212600	-1.68199900
H	-2.72629600	-5.07216100	0.35305500
H	-1.06914000	-4.67322000	-3.59837600
H	-2.69887300	-5.73913200	-2.04772400
B	2.61925600	1.71075200	0.58401300
O	2.08000700	2.03508700	1.84161600
H	2.77851700	2.25353600	2.47713600
C	4.19204700	1.83186900	0.37410800
C	4.79278600	1.10090300	-0.66715200
C	5.03665000	2.60540900	1.18906000
C	6.16951300	1.12231800	-0.88687300
H	4.15915200	0.50445200	-1.31331400
C	6.41789200	2.65488300	0.98732000
H	4.61988300	3.20299900	1.99842900
C	6.95671400	1.90402100	-0.04956200
H	6.63130500	0.54973600	-1.68539200
H	7.06903800	3.25768600	1.61266800
F	8.29912100	1.93617600	-0.25167900

5-PPh₃:**E: -3116.134436****G293: -3115.434308****G243: -3115.415243**

Pd	-0.36673200	-0.09058400	0.08762900
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P	-2.52707500	-1.03710100	0.18366200
P	1.61965300	1.18348100	0.37742100
C	-2.64763200	-2.51216800	1.27609800
C	-1.99503700	-3.68292100	0.85199100
C	-3.32392300	-2.51572000	2.50382500
C	-2.00092100	-4.82375400	1.65382100
H	-1.47194800	-3.71895000	-0.09713500
C	-3.33378500	-3.66447100	3.29801500
H	-3.85778200	-1.63557900	2.84071600
C	-2.66806400	-4.81803000	2.88063700
H	-1.47787300	-5.71294700	1.31496500
H	-3.86835700	-3.65422900	4.24375300
H	-2.67299300	-5.70724000	3.50453200
C	-3.19254600	-1.67739800	-1.39256100
C	-2.49518000	-1.45931800	-2.58683000
C	-4.38701600	-2.41575300	-1.41315500
C	-2.98809300	-1.96578500	-3.79163200
H	-1.56344100	-0.90757700	-2.56952100
C	-4.87879400	-2.91521700	-2.61729600
H	-4.92691800	-2.60004000	-0.48913400
C	-4.18011100	-2.69034100	-3.80812000
H	-2.43717300	-1.79601600	-4.71225300
H	-5.80384300	-3.48441400	-2.62718200
H	-4.56353800	-3.08553500	-4.74444400
C	-3.76954800	0.14256800	0.81563100
C	-4.83423600	0.59240900	0.02649900
C	-5.37356500	0.70177400	2.08949800
C	-5.69794700	1.57751600	0.51007500
H	-4.98562900	0.18845000	-0.96822900
C	-4.45001400	1.66869900	2.57707300
H	-2.72084200	0.39661300	2.68990700
C	-5.51295500	2.11218200	1.78551900
H	-6.51571400	1.92573300	-0.11437300
H	-4.29185900	2.08926100	3.56607200
H	-6.18806900	2.87662500	2.15933700
C	2.51849800	0.85629400	1.93898700
C	2.15313300	-0.23084500	2.74343500
C	3.54975000	1.71148500	2.36558200
C	2.82032700	-0.47028900	3.94702800
H	1.37383800	-0.90217100	2.40436100
C	4.21893100	1.46339500	3.56268200
H	3.82116200	2.57705500	1.76999500
C	3.85571600	0.37085400	4.35563200
H	2.53163700	-1.31924300	4.56054200
H	5.01868300	2.12675500	3.87942100
H	4.37604300	0.18129000	5.29035300
C	1.33998000	2.99761600	0.46996800
C	1.34361900	3.79104900	-0.68420500
C	0.98603500	3.57758800	1.69749800
C	0.99241400	5.13911300	-0.61243200
H	1.60993400	3.35882900	-1.64230000
C	0.64690100	4.92820700	1.76806100
H	0.97025400	2.97390800	2.59940100
C	0.64371500	5.71193000	0.61223400
H	0.99193600	5.74128600	-1.51658600
H	0.37836400	5.36550300	2.72576900
H	0.37072300	6.76204400	0.66520100
C	2.81991200	1.00285000	-0.99393200
C	4.20704700	0.99141500	-0.80320600
C	2.30285900	0.92533800	-2.29624100
C	5.06336500	0.93535500	-1.90304300
H	4.62419300	1.00673700	0.19622200
C	3.16248900	0.88183400	-3.39294100
H	1.23045000	0.89143200	-2.44710100
C	4.54516300	0.89349200	-3.19837300
H	6.13741400	0.91044800	-1.74315700
H	2.75138900	0.82647700	-4.39709200

H	5.21601200	0.85005700	-4.05181700
C	-1.25995000	1.59985200	-0.57008800
C	-1.36832400	1.83345100	-1.94817400
C	-1.75485900	2.57730600	0.30365900
C	-1.95581900	3.00359600	-2.44516400
H	-0.98904400	1.11084400	-2.66313100
C	-2.34990100	3.74764400	-0.16889900
H	-1.67201600	2.44000600	1.37490100
C	-2.43762400	3.93849600	-1.54165900
H	-2.03615500	3.18745100	-3.51231600
H	-2.72959100	4.50403800	0.51028900
O	0.67106400	-1.98419100	0.62776700
F	-3.00870300	5.07963200	-2.01310700
B	1.26133600	-2.68269900	-0.61721300
O	0.69508900	-2.09124500	-1.83643200
H	-0.18088500	-2.48910500	-1.95399700
O	0.83695500	-4.08066600	-0.43288400
H	1.30527400	-4.62804500	-1.07931100
C	2.87034200	-2.48997000	-0.62540200
C	3.60043100	-2.48088700	-1.82652400
C	3.61427100	-2.42153300	0.56443300
C	4.99534400	-2.40452500	-1.85303100
H	3.05936400	-2.51824300	-2.76785100
C	5.00842000	-2.32432900	0.57435100
H	3.08853400	-2.42921600	1.51340400
C	5.67250000	-2.31807600	-0.64458000
H	5.55258500	-2.38519500	-2.78477800
H	5.57243000	-2.25002300	1.49970900
F	7.03175900	-2.20982200	-0.65718100
H	0.06349000	-2.61379600	1.04826800

5-PPh₃-cis:**E: -3116.131818****G293: -3115.432016****G243: -3115.412885**

Pd	0.20115200	0.32659500	-0.13503500
P	-1.85556800	1.26746800	0.20408500
C	-2.78643900	1.47667600	-1.34854000
C	-2.33135400	0.80714200	-2.49165400
C	-3.94146000	2.27211800	-1.42863000
C	-3.03079600	0.90916600	-3.69432300
H	-1.42851000	0.20921200	-2.42948200
C	-4.63707600	2.37420100	-2.63247000
H	-4.28984400	2.81741800	-0.55749000
C	-4.18529500	1.69013600	-3.76492400
H	-2.67317600	0.37918200	-4.57203300
H	-5.52992200	2.99025500	-2.68708800
H	-4.73007400	1.77199800	-4.70113600
C	-1.81645900	2.93741900	0.96934600
C	-1.70575400	3.05934600	2.36108100
C	-1.76727600	4.09193200	0.17499800
C	-1.53853500	4.31465300	2.94716100
H	-1.74427500	2.17839500	2.99282700
C	-1.59893800	5.34403400	0.76398300
H	-1.84001000	4.01548300	-0.90301900
C	-1.48058500	5.45945000	2.15083200
H	-1.45289400	4.39470500	4.02719600
H	-1.55387800	6.22900900	0.13572000
H	-1.34412900	6.43569100	2.60726500
C	-2.92966400	0.32885300	1.35185100
C	-4.31798800	0.22829600	1.19146500
C	-2.31313800	-0.31300500	2.43435600
C	-5.07288300	-0.51685000	2.09695300
H	-4.80901700	0.69975900	0.34857100
C	-3.06934000	-1.06071000	3.33713200

H	-1.23828500	-0.24518200	2.55565600
C	-4.45073300	-1.16802000	3.16598000
H	-6.14711700	-0.60017400	1.95840900
H	-2.57392100	-1.57318800	4.15573800
H	-5.04070100	-1.75995500	3.85990100
C	0.82045900	2.24487700	-0.40872500
C	1.46402200	2.94146400	0.62466500
C	0.68921800	2.86289300	-1.65953500
C	1.93873600	4.24029300	0.42756400
H	1.60511400	2.46245400	1.58822300
C	1.16762000	4.16116500	-1.87780200
H	0.18968600	2.34994400	-2.47730500
C	1.77147500	4.82736800	-0.82131200
H	2.42962000	4.79370200	1.22236800
H	1.06355400	4.65278800	-2.84040300
F	2.21999900	6.09618000	-1.01496300
P	-0.37981000	-2.03814800	-0.19020200
O	2.26217800	-0.13437400	-0.39701400
C	0.84259800	-2.99418100	-1.17367600
C	1.47724500	-2.36760400	-2.25613500
C	1.14816000	-4.32982300	-0.88215600
C	2.40041000	-3.06642400	-3.03553000
H	1.27134300	-1.32515000	-2.47072400
C	2.08071100	-5.02348900	-1.65499600
H	0.67447000	-4.82494000	-0.04137400
C	2.70900000	-4.39472400	-2.73271900
H	2.88818900	-2.56743700	-3.86828500
H	2.31755800	-6.05564000	-1.41209500
H	3.43754200	-4.93529500	-3.33039400
C	-0.54750200	-2.94088100	1.39238600
C	-1.34748900	-4.08434600	1.52995400
C	0.15865600	-2.45485800	2.50298000
C	-1.45394400	-4.72381200	2.76617700
H	-1.89531700	-4.47305400	0.67804600
C	0.05246900	-3.09956000	3.73496300
H	0.79637300	-1.58471900	2.39062300
C	-0.75696600	-4.23068100	3.87125600
H	-2.08048500	-5.60599900	2.86343800
H	0.60029300	-2.71573100	4.59149700
H	-0.84289500	-4.72700200	4.83404000
C	-1.94650300	-2.38820300	-1.09592700
C	-3.18129100	-2.35514400	-0.43057700
C	-1.93531600	-2.57344400	-2.48719600
C	-4.37418100	-2.48346600	-1.14222700
H	-3.21588900	-2.24044800	0.64447100
C	-3.12950600	-2.70279100	-3.19636000
H	-0.99362800	-2.61473700	-3.02367300
C	-4.35409500	-2.65078000	-2.52773100
H	-5.31892200	-2.45072800	-0.60718300
H	-3.10037800	-2.84500600	-4.27311200
H	-5.28405200	-2.74675000	-3.08091400
B	3.03320800	-0.65247700	0.83941600
O	2.49031800	0.05363700	2.00464000
H	2.82223500	-0.39075000	2.79912300
O	2.76865700	-2.07052400	0.97729100
H	3.06201400	-2.54073000	0.18451500
C	4.60092300	-0.29840800	0.53127900
C	5.30960800	-0.94296700	-0.50021100
C	5.30193300	0.66901200	1.26862700
C	6.64509800	-0.65148700	-0.78635300
H	4.80801500	-1.69618300	-1.10704200
C	6.64020800	0.98459000	1.01082100
H	4.78098000	1.19020200	2.06811900
C	7.28610100	0.31279900	-0.01743100
H	7.18656100	-1.15223100	-1.58372300
H	7.17687000	1.73304700	1.58676100
F	8.58841800	0.60737300	-0.28408900

H	2.65871200	0.71176600	-0.65964900
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8-PPh₃:

E: -3143.301901

G293: -3142.622784

G243: -3142.603694

Pd	1.44520800	0.73081700	0.89008600
P	2.95955700	-0.73883500	0.09109000
C	3.65439900	-1.78112800	1.42517500
C	2.84029100	-2.08284900	2.52907600
C	4.94985500	-2.31319500	1.35178200
C	3.32188800	-2.90968300	3.54409500
H	1.83410400	-1.67442600	2.57925300
C	5.42661900	-3.13577100	2.37378500
H	5.58544600	-2.08560500	0.50234700
C	4.61475100	-3.43435600	3.47028200
H	2.68808000	-3.13849400	4.39637700
H	6.43251100	1.31567500	2.31223200
H	4.98939800	-4.07255800	4.26568600
C	4.40885200	-0.09010000	-0.81067700
C	4.57088300	-0.28309500	-2.18690300
C	5.32636100	0.71127600	-0.11125700
C	5.63284400	0.32804300	-2.85937500
H	3.87027200	-0.90135200	-2.73813200
C	6.38417000	1.31567500	-0.78413000
H	5.19976200	0.87595800	0.95388500
C	6.53648100	1.12965100	-2.16226500
H	5.75006300	0.17497600	-3.92854900
H	7.08326500	1.94090500	-0.23643400
H	7.35710900	1.60961400	-2.68785500
C	2.17236100	-1.92152700	-1.06500500
C	2.54262100	-3.27226100	-1.12188600
C	1.19470200	-1.43560100	-1.94681800
C	1.94847700	-4.12002900	-2.05800000
H	3.29134500	-3.66156700	-0.43970600
C	0.61127500	-2.28253100	-2.88861000
H	0.89390900	-0.39489400	-1.88722600
C	0.99015300	-3.62582600	-2.94573100
H	2.23612500	-5.16690100	-2.09349100
H	-0.14390800	-1.89502000	-3.56503700
H	0.53134700	-4.28884800	-3.67374000
C	2.56354900	2.30851200	0.38948200
C	2.73475700	2.70122500	-0.94941100
C	3.18823100	3.08042800	1.38309000
C	3.51128100	3.81106200	-1.29474300
H	2.28328800	2.11936400	-1.74896000
C	3.97713900	4.19072700	1.05917900
H	3.07584900	2.81125700	2.43050100
C	4.12560300	4.53100600	-0.27836900
H	3.65267700	4.10797300	-2.32968900
H	4.47022700	4.78181100	1.82540400
F	4.89777000	5.60325400	-0.60460500
Pd	-1.52296800	0.59522000	1.01177500
P	-2.86515700	-0.82960400	-0.10618700
C	-2.76968200	-0.52425000	-1.90593100
C	-1.75637800	0.30777500	-2.40087800
C	-3.67473900	-1.11624900	-2.80035500
C	-1.63869700	0.53657900	-3.77247500
H	-1.06762200	0.77446400	-1.70339900
C	-3.55243200	-0.89048800	-4.17130800
H	-4.47269600	-1.75053900	-2.42641200
C	-2.53470500	-0.06499800	-4.65901300
H	-0.85080900	1.18479400	-4.14552200
H	-4.25447300	-1.35389400	-4.85846100
H	-2.44576600	0.11334600	-5.72689200

C	-4.66388000	-0.84491400	0.23923900
C	-5.26162700	-1.85235400	1.00737800
C	-5.45002600	0.21949800	-0.23334800
C	-6.62584800	-1.79469700	1.30172400
H	-4.67080900	-2.68548600	1.37246500
C	-6.81115900	0.26980000	0.05944400
H	-4.99870300	1.00921400	-0.82401500
C	-7.40219200	-0.73511900	0.83036600
H	-7.07956300	-2.58289700	1.89590400
H	-7.40777200	1.09909900	-0.30960200
H	-8.46305300	-0.69225300	1.06028900
C	-2.29982800	-2.55442600	0.14229300
C	-2.04256800	-3.42924300	-0.92083500
C	-2.06325500	-2.98484000	1.46015200
C	-1.56308000	-4.71631300	-0.67002100
H	-2.20101500	-3.10785100	-1.94323900
C	-1.59738300	-4.27525500	1.70637300
H	-2.22677900	-2.30167000	2.28737800
C	-1.34264700	-5.14248800	0.64029600
H	-1.35557500	-5.38213100	-1.50225300
H	-1.41953600	-4.59693900	2.72845700
H	-0.96614000	-6.14336400	0.83127000
C	-2.87688600	2.04703000	0.76335000
C	-3.85761700	2.25072000	1.74963400
C	-2.86180900	2.91803400	-0.33741800
C	-4.79619100	3.28156300	1.64663100
H	-3.91070500	1.58451600	2.60712000
C	-3.79738700	3.95233800	-0.46408400
H	-2.12471000	2.79039900	-1.12480600
C	-4.75015900	4.11032300	0.53297800
H	-5.55885700	3.43487100	2.40427000
H	-3.79149800	4.62320900	-1.31818800
F	-5.66909500	5.10657700	0.41464300
O	-0.05824100	1.89494100	1.79979500
H	-0.13201000	2.77205300	1.38991000
O	0.05268300	-0.77540000	1.46519000
H	0.04039400	-1.53171900	0.85773100

9-PPh₃:

E: -3651.087912

G293: -3650.295596

G243: -3650.273995

B	-0.71474300	2.26167500	-0.76075600
Pd	1.70539900	0.13404200	-1.16594300
Pd	-1.48247100	-0.70835200	-1.07480000
O	0.70186700	2.09255600	-1.32216500
O	-1.54118900	1.41001700	-1.69526700
O	0.17779900	-0.66200600	-2.40205300
H	1.26368700	2.78518300	-0.93883900
H	-1.06174800	1.35243400	-2.53909600
H	0.45245100	-1.58037900	-2.56204100
C	-1.13699800	3.81633800	-0.79357300
C	-1.99038900	4.34973700	-1.77138000
C	-0.62809500	4.70709800	0.16800400
C	-2.32967100	5.70557700	-1.80184000
H	-2.41307600	3.68715800	-2.52132700
C	-0.94253400	6.06801000	0.16144300
H	0.02607500	4.32804700	0.94785300
C	-1.79332900	6.53987400	-0.83019000
H	-2.99632900	6.11448900	-2.55532100
H	-0.54640800	6.75302800	0.90524900
C	2.55064900	-1.68145200	-1.27681000
C	3.02270600	-2.09085000	-2.53759100
C	2.55280700	-2.61817200	-0.23523900
C	3.49377900	-3.39022900	-2.75297800

H	3.02797300	-1.39409100	-3.37215600
C	3.01292500	-3.92392500	-0.43384800
H	2.16943800	-2.35405000	0.74109000
C	3.47915300	-4.28350800	-1.69026900
H	3.86222600	-3.70696100	-3.72405200
H	2.98640800	-4.65924200	0.36396900
C	-1.06749400	-2.57682200	-0.49084900
C	-0.93849700	-3.60512200	-1.44016300
C	-0.68692700	-2.84936700	0.83249900
C	-0.43875700	-4.86305000	-1.08685800
H	-1.21909100	-3.43465000	-2.47678500
C	-0.18992800	-4.10115000	1.20539700
H	-0.75198300	-2.92083200	1.59168500
C	-0.07089600	-5.08369500	0.23360100
H	-0.32386000	-5.65485000	-1.82069800
H	0.12542700	-4.30227300	2.22470200
F	-2.11360000	7.86268200	-0.84798900
F	0.44423600	-6.29338800	0.58062800
F	3.92501300	-5.55191400	-1.89052300
O	-0.79211700	1.76368400	0.59911200
H	-0.45820900	0.84977400	0.58961100
P	-3.36064300	-0.65880200	0.20076900
P	3.24678800	0.79963300	0.35721600
C	-3.08463800	-0.97769700	1.97838800
C	-3.49756000	-2.17286700	2.58138600
C	-2.33227400	-0.05144800	2.72137100
C	-3.17443200	-2.43412500	3.91435200
H	-4.06017200	-2.90539900	2.01364600
C	-2.02467000	-0.31296100	4.05631300
H	-1.98427300	0.86279700	2.25045600
C	-2.44218800	-1.50548100	4.65543500
H	-3.49626200	-3.36574600	4.37087300
H	-1.45316800	0.41417600	4.62634500
H	-2.19538400	-1.70919800	5.69357700
C	3.04520400	-0.18715600	1.88251600
C	4.08520200	-0.96210100	2.40891300
C	1.75926100	-0.28823200	2.44190400
C	3.84340200	-1.82640300	3.47929700
H	5.07742000	-0.91212600	1.97520200
C	1.52385500	-1.14667200	3.51356400
H	0.94153900	0.29485100	2.03205000
C	2.56544900	-1.92332800	4.03020400
H	4.65559700	-2.43039900	3.87343500
H	0.52514900	-1.22031700	3.93165800
H	2.37780600	-2.60346400	4.85611700
C	-4.66039500	-1.83656300	-0.31784300
C	-5.91005900	-1.83129600	0.32317000
C	-4.43700400	-2.71057100	-1.38798400
C	-6.91189100	-2.70623800	-0.09080500
H	-6.09653500	-1.14360400	1.14281200
C	-5.44563600	-3.58291700	-1.80435400
H	-3.47733700	-2.70326000	-1.89158100
C	-6.68011200	-3.58477700	-1.15452100
H	-7.87462400	-2.70060700	0.41219700
H	-5.26395000	-4.25810400	-2.63570000
H	-7.46406300	-4.26395300	-1.47739200
C	5.02122200	0.73849300	-0.06951200
C	5.96624400	1.30628000	0.80198500
C	5.44788000	0.16364900	-1.27198700
C	7.32077500	1.27855900	0.47795300
H	5.64221500	1.76885300	1.72966200
C	6.80655300	0.14242100	-1.59524000
H	4.72100300	-0.26685400	-1.94910200
C	7.74279300	0.69530500	-0.72122800
H	8.04662800	1.71539500	1.15772800
H	7.12907900	-0.30518500	-2.53090900
H	8.79929100	0.67813600	-0.97327800

C	3.03912400	2.55534100	0.84803600
C	2.65127400	2.95427500	2.13184500
C	3.27728900	3.53229200	-0.13603400
C	2.50132100	4.31190600	2.42708200
H	2.47091600	2.21474700	2.90378000
C	3.11928300	4.88492900	0.16208900
H	3.59947600	3.23334400	-1.13105500
C	2.73075800	5.27719400	1.44602700
H	2.20250400	4.61153700	3.42748000
H	3.29859300	5.63008600	-0.60711200
H	2.60518400	6.33071400	1.67770300
C	-4.23228300	0.94967000	0.10107000
C	-4.67202600	1.65622400	1.22662000
C	-4.49617500	1.45942800	-1.17958300
C	-5.34908700	2.86822500	1.07233600
H	-4.48970300	1.27044300	2.22291100
C	-5.17894700	2.66400500	-1.32899200
H	-4.15153200	0.92093300	-2.05571500
C	-5.59982100	3.37598300	-0.20241400
H	-5.67957500	3.41269300	1.95243500
H	-5.37078400	3.05410800	-2.32444900
H	-6.12004600	4.32235000	-0.31978500

H	-6.00365600	0.37107000	-0.00001900
H	-4.72441700	-3.72405500	-0.00029100
C	0.64215200	2.86491700	0.00008100
C	1.97876800	3.30572200	-0.00003500
C	-0.37780500	3.83473600	-0.00001200
C	2.29609100	4.66176600	-0.00015400
H	2.78165800	2.57450000	0.00004200
C	-0.08507700	5.19633800	-0.00010300
H	-1.41622000	3.51698100	0.00008900
C	1.25172400	5.58038500	-0.00017200
H	3.32283000	5.01268000	-0.00023600
H	-0.86334000	5.95242500	-0.00016700
C	2.16026300	-1.98912600	0.00015500
C	1.87496100	-3.36730600	-0.00023600
C	3.50985000	-1.58970500	0.00040400
C	2.89143200	-4.31934000	-0.00038500
H	0.84065300	-3.69800900	-0.00038400
C	4.54345000	-2.52313400	0.00026700
H	3.75308900	-0.53138900	0.00073600
C	4.20878400	-3.87314100	-0.00012900
H	2.68287300	-5.38415800	-0.00071800
H	5.58707500	-2.22625800	0.00047400
F	5.20368000	-4.78818300	-0.00030200
F	-6.74989800	-2.10947000	-0.00024600
F	1.54784400	6.89927300	-0.00031900

OTHER COMPOUNDS

THF:

E: -232.565096

G293: -232.472014

G243: -232.46717

C	1.16535400	-0.42701800	-0.13350000
O	-0.00009100	-1.25402700	-0.00025600
C	-1.16533200	-0.42689300	0.13382200
C	-0.73151400	0.99451200	-0.23156100
C	0.73154500	0.99455000	0.23142000
H	1.95280200	-0.82021900	0.52030700
H	1.52928300	-0.47350000	-1.17149400
H	-1.95325100	-0.82015600	-0.51936500
H	-1.52851500	-0.47318000	1.17209800
H	-0.78638000	1.14398800	-1.31653600
H	-1.34490700	1.76006800	0.25291900
H	1.34497500	1.75992000	-0.25330700
H	0.78640700	1.14438900	1.31634100

7:

E: -1293.859867

G293: -1293.626033

G243: -1293.615486

B	1.02133400	-0.94116700	0.00017700
O	1.31208500	0.40998900	0.00022800
B	0.30342900	1.35478300	0.00018000
O	-0.30124700	-1.34245200	0.00022600
B	-1.32596500	-0.41494000	0.00026200
O	-1.01205300	0.93100200	0.00033200
C	-2.80321800	-0.87645600	0.00017400
C	-3.85334600	0.06062200	0.00016900
C	-3.13316900	-2.24464000	-0.00001000
C	-5.18638300	-0.34264100	0.00002900
H	-3.62175400	1.12156600	0.00026400
C	-4.45864100	-2.67204900	-0.00014300
H	-2.33867300	-2.98486200	-0.00005900
C	-5.45967400	-1.70640900	-0.00011700

P(iPr)₃:

E: -697.1926245

G293: -696.9412855

G243: -696.9333525

P	0.14602700	0.08287300	-0.76784900
C	-0.85041700	1.45205400	0.06746600
H	-0.18608200	2.31631000	-0.06726800
C	1.77022200	0.14835000	0.18257900
H	1.57258200	0.00527200	1.25207800
C	-0.55824000	-1.58694600	-0.22071600
H	0.03018700	-2.28325500	-0.83481900
C	2.45759800	1.50764200	-0.00352900
H	3.44655000	1.49814000	0.47291100
H	2.60331100	1.73816700	-1.06654800
H	1.88690100	2.32767900	0.44395200
C	2.69106900	-0.98044400	-0.30300400
H	2.89920300	-0.88195200	-1.37593100
H	3.65129500	-0.94292900	0.22753700
H	2.26017600	-1.97304700	-0.13661900
C	-2.02263500	-1.73136400	-0.65868600
H	-2.17413700	-1.41770900	-1.69805600
H	-2.34222300	-2.77802700	-0.57332700
H	-2.68740600	-1.13454000	-0.02510600
C	-0.38593000	-2.01274900	1.24307500
H	-0.99011600	-1.40265300	1.91956700
H	-0.71031600	-3.05560000	1.36284400
H	0.65440000	-1.95555000	1.57681200
C	-2.13328900	1.76469200	-0.71851200
H	-2.87947300	0.97065300	-0.61448700
H	-2.58770700	2.69218200	-0.34572000
H	-1.92962200	1.89579300	-1.78727200
C	-1.14062100	1.31627800	1.56589300
H	-1.53658500	2.26212200	1.96050900
H	-1.89354800	0.54455100	1.75631800
H	-0.24434000	1.06621000	2.14296200

Pd-P(iPr)₃:

E: -825.2000135

G293: -824.9506115**G243: -824.9418295**

Pd	-1.91778600	-0.41966000	-0.14834000
P	0.22895600	0.11308300	0.02570100
C	1.06984600	-0.69120600	1.50476500
H	0.57472800	-0.17979500	2.33987200
C	0.55173600	1.94039600	0.29596900
H	1.63815800	2.08075600	0.34598600
C	1.20475000	-0.26461600	-1.54361900
H	0.55698400	0.17519400	-2.31248000
C	-0.06395800	2.42777100	1.61269600
H	0.07899700	3.51127100	1.71167400
H	-1.14164100	2.22379700	1.63808600
H	0.39175700	1.95437400	2.48788300
C	0.00110200	2.75233600	-0.88346200
H	-1.08342100	2.61333100	-0.97197100
H	0.19652500	3.82072900	-0.72743400
H	0.45459800	2.46652800	-1.83778000
C	1.26798100	-1.77370700	-1.81115600
H	0.28491000	-2.24476800	-1.69842400
H	1.61876900	-1.95653300	-2.83463000
H	1.96651700	-2.27141100	-1.13052700
C	2.59250200	0.37595900	-1.68228600
H	3.31167800	-0.04299100	-0.97399000
H	2.97653700	0.18413000	-2.69277300
H	2.57148400	1.46058000	-1.54286100
C	0.72276600	-2.18069700	1.63277000
H	1.19872500	-2.77945800	0.85026100
H	1.07293100	-2.56084800	2.60116700
H	-0.35929700	-2.34059900	1.57005700
C	2.58035300	-0.46288000	1.63592100
H	2.91600900	-0.78706800	2.62954300
H	3.13653100	-1.04836400	0.89717800
H	2.85987000	0.58909600	1.51970700

Pd-(P(iPr)₃)₂:**E: -1522.457338****G293: -1521.934894****G243: -1521.92138**

Pd	0.00000000	0.04863100	0.00003800
P	2.31439400	0.05734000	-0.04891200
P	-2.31441600	0.05744900	0.04890200
C	-3.02701100	-1.47299300	0.88280200
H	-2.42887300	-1.51577200	1.80243300
C	-3.08783000	0.26881900	-1.65092600
H	-2.81596000	1.30596600	-1.88589500
C	-3.05333600	1.46718900	1.03801900
H	-4.14589600	1.37546800	1.01365900
C	3.08782900	0.26930100	1.65080200
H	2.81554200	1.30638800	1.88556500
C	3.02698000	-1.47335400	-0.88236200
H	2.42880100	-1.51644700	-1.80195100
C	3.05319000	1.46675500	-1.03859800
H	4.14573900	1.37485600	-1.01469400
C	2.66248000	2.82182000	-0.43525800
H	3.03192900	3.63547300	-1.07251800
H	1.57183500	2.91538100	-0.36285100
H	3.08236100	2.97027900	0.56466100
C	2.57787100	1.37809800	-2.49539100
H	1.48330500	1.43343700	-2.54505200
H	2.98866400	2.21286100	-3.07747900
H	2.88909000	0.44816600	-2.98196500
C	2.70419700	-2.73800200	-0.07569300
H	1.65185600	-2.76238500	0.22985800

H	2.90466200	-3.63063800	-0.68182900
H	3.32391500	-2.80615800	0.82468200
C	4.50552700	-1.44039500	-1.28951200
H	5.16969000	-1.45374600	-0.42138400
H	4.73570500	-2.32830100	-1.89316500
H	4.75504800	-0.56247200	-1.89288700
C	2.39592100	-0.61191900	2.70104900
H	2.63236700	-1.67177500	2.56487500
H	2.72794200	-0.32413700	3.70720700
H	1.30680200	-0.50098000	2.65064900
C	4.61288100	0.14893800	1.73733900
H	4.95828200	0.49786200	2.71941400
H	4.93636500	-0.89126100	1.62889800
H	5.12403700	0.74598200	0.97509900
C	-2.66210600	2.82204000	0.43452200
H	-3.03183900	3.63592100	1.07132300
H	-1.57140400	2.91542300	0.36274900
H	-3.08134400	2.97027500	-0.56570200
C	-2.57856700	1.37883100	2.49500400
H	-1.48400700	1.43404100	2.54502800
H	-2.98942900	2.21381700	3.07672200
H	-2.89006900	0.44908000	2.98173600
C	-4.50558300	-1.44003400	1.28987200
H	-5.16971100	-1.45407200	0.42172700
H	-4.73561300	-2.32759700	1.89408300
H	-4.75530900	-0.56176900	1.89266700
C	-2.70408100	-2.73786800	0.07654100
H	-1.65170900	-2.76227700	-0.22889700
H	-2.90455400	-3.63033300	0.68292900
H	-3.32369900	-2.80633800	-0.82387800
C	-2.39553700	-0.61237200	-2.70094300
H	-2.63157400	-1.67228800	-2.56451300
H	-2.72763000	-0.32497000	-3.70718500
H	-1.30646400	-0.50099800	-2.65052000
C	-4.61283500	0.14785900	-1.73749000
H	-4.95832700	0.49644100	-2.71965400
H	-4.93594200	-0.89242900	-1.62882100
H	-5.12421600	0.74489800	-0.97539300

Pd-(P(iPr)₃)₃:**E: -2219.684334****G293: -2218.886653****G243: -2218.868756**

Pd	0.00017400	-0.00001200	0.04035400
P	0.09838500	-2.36386600	0.05672700
P	1.99758000	1.26675200	0.05580100
P	-2.09575600	1.09627100	0.05725200
C	-3.07144700	0.86048200	1.65006300
H	-4.00023200	1.43745100	1.57633300
C	-3.27198300	0.40136100	-1.24257100
H	-3.38755700	-0.63124300	-0.89127400
C	-2.14528300	2.98810500	-0.10934600
H	-1.31105400	3.28557300	0.53550500
C	-2.59930200	0.31794300	-2.62087000
H	-1.59163100	-0.10422900	-2.54277600
H	-3.18874300	-0.32225100	-3.29083300
H	-2.51674700	1.30062600	-3.09417100
C	-4.66766900	1.02414300	-1.34686500
H	-5.30325500	0.41296300	-2.00254100
H	-5.16741100	1.09335200	-0.37495600
H	-4.62631900	2.02874600	-1.78001500
C	-2.24778500	1.39477500	2.82982900
H	-2.80263800	1.27418000	3.76984300
H	-1.30487900	0.84197500	2.91710700
H	-2.00176900	2.45607200	2.72259100

C	-3.43746100	-0.60619700	1.89371500
H	-2.53630900	-1.22319300	1.95090800
H	-3.97549300	-0.70444000	2.84620800
H	-4.08142900	-1.01407900	1.10808900
C	-1.78664500	3.42960200	-1.53374100
H	-2.63588200	3.30536900	-2.21410600
H	-1.51418800	4.49321100	-1.54250900
H	-0.94368300	2.86216600	-1.93562500
C	-3.39096200	3.73756900	0.38327300
H	-3.23394500	4.81910900	0.26757300
H	-4.28614400	3.47559500	-0.18736500
H	-3.59989700	3.55469700	1.44119100
C	1.28651200	-3.03045800	-1.24692700
H	2.23922300	-2.61509300	-0.89574900
C	-1.51601600	-3.35151300	-0.10802700
H	-2.18835300	-2.77872000	0.54028200
C	0.79400300	-3.09491600	1.64590700
H	0.76300300	-4.18764100	1.56693000
C	-0.08161700	-2.65809200	2.82823000
H	0.30037500	-3.08444900	3.76544400
H	-0.07583300	-1.56579000	2.92351800
H	-1.12322600	-2.97637000	2.71818000
C	2.24571300	-2.67340700	1.88973300
H	2.32623100	-1.58429400	1.94998700
H	2.60202300	-3.09172800	2.84075500
H	2.92149200	-3.02271600	1.10256900
C	1.02079900	-2.40192300	-2.62296700
H	0.12950900	-2.82214300	-3.09749300
H	0.87936100	-1.31890100	-2.54103500
H	1.87033300	-2.58803400	-3.29362700
C	1.44605400	-4.55035300	-1.35556300
H	2.29339500	-4.79288400	-2.01180100
H	1.63611100	-5.02047500	-0.38498000
H	0.55591000	-5.01627600	-1.78961000
C	-2.08140900	-3.25751200	-1.53074600
H	-3.13877500	-3.55373700	-1.53778600
H	-2.01317300	-2.24276100	-1.93018400
H	-1.55002200	-3.92821600	-2.21447200
C	-1.54116600	-4.80674900	0.37988400
H	-2.55690200	-5.21084700	0.26662700
H	-0.86903400	-5.44923100	-0.19564900
H	-1.27434200	-4.90002000	1.43651700
C	3.66077300	0.36312600	-0.10960100
H	3.50130300	-0.50596500	0.53817500
C	2.28525400	2.23648100	1.64405100
H	3.24694300	2.75577600	1.56303400
C	1.97885400	2.62856400	-1.24831800
H	1.14377400	3.24631200	-0.89527000
C	4.93282800	1.06901500	0.37994300
H	5.79155100	0.39316800	0.26335700
H	5.15106600	1.97478500	-0.19237400
H	4.88073100	1.34281500	1.43759100
C	3.86413800	-0.17204100	-1.53263800
H	4.17936500	0.62456400	-2.21504000
H	4.65026600	-0.93868900	-1.53958800
H	2.95257300	-0.62121100	-1.93422400
C	2.34664800	1.26152700	2.82766600
H	2.52962000	1.80659500	3.76332400
H	1.39671800	0.72309200	2.92718600
H	3.14086200	0.51653100	2.71587700
C	1.19553000	3.28380800	1.88927000
H	1.15869200	4.04299100	1.10151800
H	0.21259500	2.80819300	1.95173900
H	1.38144600	3.80254100	2.83938100
C	1.56416000	2.08273900	-2.62267500
H	1.30010500	2.91049700	-3.29433100
H	2.37243900	1.51919600	-3.09785300

H	0.69635700	1.42005300	-2.53703900
C	3.21577700	3.52543200	-1.35985600
H	3.00228400	4.37980400	-2.01711000
H	3.52900400	3.92591800	-0.38993500
H	4.06360400	2.98584300	-1.79413100

4:

E: -507.7598384

G293: -507.6726944

G243: -507.6664004

B	-2.20808100	-0.00003900	-0.00004700
O	-2.94491800	1.09546500	-0.36787200
H	-2.38324000	1.81102400	-0.70161400
O	-2.94491900	-1.09535300	0.36804400
H	-2.38306100	-1.81087100	0.70159600
C	-0.63606600	-0.00020400	-0.00017000
C	0.09326600	1.18637100	0.20022100
C	0.09346400	-1.18660600	-0.20039200
C	1.48720600	1.19981000	0.20761200
H	-0.42987300	2.12451900	0.37201300
C	1.48742700	-1.19979500	-0.20762000
H	-0.42949200	-2.12486000	-0.37218500
C	2.15708700	0.00005300	0.00003200
H	2.05111400	2.11232600	0.37116200
H	2.05148300	-2.11222900	-0.37110000
F	3.50976400	0.00017900	0.00009700

4-THF:

E: -740.339911

G293: -740.140120

G243: -740.131698

B	0.02145600	-0.00330900	0.27489600
O	0.80590000	1.12989700	0.17178400
H	0.29371900	1.92415800	-0.04185300
O	0.62533500	-1.19684300	0.50070300
H	1.61368300	-1.12943100	0.52793600
C	-1.54413500	0.03592200	0.13719400
C	-2.27996600	1.23420500	0.13634100
C	-2.26321300	-1.16696600	0.00814600
C	-3.66895900	1.24667200	0.00981600
H	-1.77581300	2.19216600	0.24886200
C	-3.65062900	-1.18445100	-0.12411700
H	-1.72070000	-2.10743800	0.01105900
C	-4.32672600	0.02998800	-0.12083700
H	-4.23765800	2.17083400	0.01323700
H	-4.20625000	-2.11106700	-0.22705700
F	-5.67493000	0.02786300	-0.24744400
C	3.86714300	0.10012100	1.11827200
O	3.32426600	-1.03100900	0.39064700
C	3.60221400	-0.87971800	-1.02049300
C	3.96175700	0.58981800	-1.21519300
C	4.68005000	0.90787700	0.10414700
H	3.03083300	0.68307900	1.51776800
H	4.46676400	-0.28448100	1.94950100
H	4.43800500	-1.53998400	-1.28872400
H	2.71298000	-1.19686700	-1.57314600
H	4.58450900	0.75426200	-2.09933800
H	3.04936400	1.18745100	-1.30381100
H	5.71586800	0.55090400	0.06941700
H	4.69255700	1.97502000	0.34392800

Boronate $p\text{-FC}_6\text{H}_4\text{B}(\text{OH})_3^-$:**E: -583.7451912****G293: -583.6493112****G243: -583.6423062**

B	-1.98439200	-0.01582000	0.00849300
C	-0.33996900	-0.00877800	-0.02763600
C	0.41149900	-1.19792200	-0.01009800
C	0.39790000	1.18699000	-0.03739400
C	1.81027700	-1.21108800	0.01136100
H	-0.11849400	-2.14803900	-0.02328700
C	1.79750000	1.21668700	-0.01821200
H	-0.15215900	2.12497500	-0.07062500
C	2.47787300	0.00706100	0.00839300
H	2.37992500	-2.13677900	0.02451900
H	2.35684100	2.14871300	-0.02866700
F	3.84509100	0.01382400	0.02508300
O	-2.53909000	1.31650300	-0.37184700
H	-2.66777400	1.27104700	-1.32974800
O	-2.43205800	-1.07111200	-0.93313000
H	-3.30663400	-1.32935700	-0.60407800
O	-2.45166000	-0.28640300	1.38821400
H	-3.12357800	0.39452200	1.53929100

H₂O:**E: -76.47019716****G293: -76.46360916****G243: -76.46072716**

O	0.00000000	0.00000000	0.12050300
H	0.00000000	0.76097200	-0.48201200
H	0.00000000	-0.76097200	-0.48201200

H₂O-THF:**E: -309.0446451****G293: -308.9310211****G243: -308.9249981**

O	2.50085600	-0.14574700	0.55102600
H	1.76279000	-0.33675500	-0.06587300
H	2.91263400	0.64666900	0.17282100
C	-0.67633400	-1.23796800	-0.12330900
O	0.16680200	-0.42899000	-0.97975000
C	-0.26019300	0.94035500	-0.86545800
C	-0.74147000	1.07009000	0.57458700
C	-1.47721800	-0.26660400	0.76693800
H	-1.32649300	-1.86218500	-0.74758800
H	-0.01820900	-1.89418100	0.45532400
H	0.59493200	1.57413100	-1.11714900
H	-1.07082400	1.14045200	-1.58180600
H	0.12817300	1.12908500	1.23739300
H	-1.37932500	1.94331300	0.73858800
H	-1.50368500	-0.59239200	1.81036900
H	-2.50996100	-0.18548000	0.41116600

B(OH)₃:**E: -252.623114****G293: -252.598306****G243: -252.593733**

B	-0.00877200	-0.02793800	0.00012900
O	1.06001100	-0.89084100	-0.00023200
H	1.91859500	-0.44292600	0.00107100
O	-1.25128600	-0.60566200	0.00013900

H	-1.94010100	0.07638500	-0.00058600
O	0.07659100	1.34838800	-0.00007600
H	0.98283600	1.69115400	0.00022200

Trimeric BO₂H:**E: -528.4522748****G293: -528.4082988****G243: -528.4022058**

B	0.41171500	-1.31613900	-0.00002300
B	-1.34586900	0.30149000	0.00005100
B	0.93404000	1.01474100	0.00002000
O	0.85076000	-2.60070200	-0.00018600
H	0.10521000	-3.22279700	-0.00011600
O	-2.67780300	0.56379300	-0.00015100
H	-2.84406000	1.52043400	0.00008100
O	1.82730900	2.03684600	-0.00014000
H	2.73871900	1.70190800	0.00036500
O	1.34967000	-0.30307300	0.00014300
O	-0.93764200	-1.01730500	0.00025600
O	-0.41220700	1.32044100	0.00000600

Boronate-H₂O:**E: -660.2336993****G293: -660.1126273****G243: -660.0828713**

B	-1.61698900	-0.66167100	-0.00887400
C	-0.01603800	-0.34290800	-0.00271400
C	0.47840300	0.97533400	0.03367800
C	0.93961900	-1.36935100	-0.04404300
C	1.84665000	1.26128800	0.03477100
H	-0.23428000	1.79725200	0.05319100
C	2.31757800	-1.11994600	-0.04124100
H	0.59002800	-2.39890400	-0.08277100
C	2.74300200	0.19986500	-0.00038000
H	2.22158400	2.28106300	0.06159400
H	3.04994100	-1.92227600	-0.07175300
F	4.08310400	0.46494700	0.00303100
O	-1.94957600	-2.09834000	-0.02231200
H	-1.79748300	-2.42591000	0.87597500
O	-2.17608000	-0.03172600	1.24266200
H	-3.10941500	-0.29909900	1.27775400
O	-2.19684300	-0.07572300	-1.25022800
H	-3.03930200	-0.53612000	-1.39081700
O	-2.58389100	2.39517400	-0.03651700
H	-2.50668500	1.72819200	-0.75450000
H	-2.44153100	1.75886700	0.69915700

Boronate-(H₂O)₂:**E: -736.7160067****G293: -736.5737267****G243: -736.5651787**

B	-1.45639900	0.01692300	0.40941800
C	0.16320400	0.11268200	0.22481800
C	0.88069500	-0.86454900	-0.49105500
C	0.91061400	1.16812900	0.76784000
C	2.26700300	-0.80268500	-0.65748600
H	0.33790300	-1.70481100	-0.91839800
C	2.29895200	1.26712000	0.61402600
H	0.38264800	1.93518000	1.32993900

C	2.95013200	0.27199900	-0.10022900
H	2.81670200	-1.56179700	-1.20771700
H	2.86969500	2.09104900	1.03398000
F	4.30441900	0.34817500	-0.25995700
O	-2.03449300	1.09583800	1.21376800
H	-2.18728200	1.84881300	0.61704800
O	-2.03511800	0.01445500	-0.99515400
H	-2.88251800	-0.45458600	-0.93123900
O	-1.78689700	-1.26449600	1.09118600
H	-2.61002300	-1.10234300	1.57696500
O	-1.26582200	-3.55900500	-0.28118700
H	-1.55597800	-2.72619300	0.17205900
H	-0.39653300	-3.70965500	0.12113400
O	-2.74244800	2.59917400	-1.20179900
H	-3.68210900	2.51632000	-0.97174500
H	-2.45565800	1.64592100	-1.29149200

Boronate-(H₂O)₃:

E: -813.2146854

G293: -813.0434634

G243: -813.0347194

B	-0.60945200	0.00940000	0.04266900
C	1.03310300	0.00677700	-0.01170200
C	1.76635200	-1.19393400	0.01730400
C	1.78395600	1.19540000	-0.03556600
C	3.16371500	-1.22375800	0.01960400
H	1.22432600	-2.13700500	0.03397400
C	3.18263700	1.20466000	-0.03156300
H	1.25649300	2.14649400	-0.06360800
C	3.84639200	-0.01423200	-0.00377700
H	3.72050800	-2.15640200	0.03913500
H	3.75319200	2.12895500	-0.05180200
F	5.20930900	-0.02505300	-0.00299200
O	-1.12626600	1.28827800	-0.54070500
H	-0.71510900	1.43834800	-1.40491100
O	-1.13889500	-1.20270200	-0.63171300
H	-0.62409600	-1.35949000	-1.43599000
O	-1.12602200	-0.05822300	1.42494700
H	-0.98729700	0.81673400	1.81728500
O	-3.83553600	-1.18991700	-1.14457400
H	-2.85521800	-1.26595000	-1.02055200
H	-3.95338500	-0.21087400	-1.16652000
O	-3.86087700	1.51934500	-0.48678600
H	-2.87269900	1.52281200	-0.56281600
H	-3.98510400	1.04631500	0.37009700
O	-3.86203600	-0.40656000	1.53596800
H	-3.98333500	-0.91628000	0.70058700
H	-2.87465900	-0.32641200	1.57580400

OH⁻:

E: -75.9137733

G293: -75.9189713

G243: -75.9163923

O	0.00000000	0.00000000	0.10941900
H	0.00000000	0.00000000	-0.87535500

[OH(H₂O)]⁻:

E: -152.4206447

G293: -152.4128847

G243: -152.4086247

O	-1.22718900	-0.07084900	-0.08211600
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H	-1.40701600	0.62551600	0.57117300
O	1.22489900	-0.07032600	0.08195700
H	0.01984200	-0.11943200	0.00335000
H	1.40549300	0.62330900	-0.57324900

[OH(H₂O)₂]⁻:

E: -228.9164271

G293: -228.8829261

G243: -228.8777531

O	-1.38028600	0.75625300	0.00907100
H	-2.32561800	0.54411700	-0.01287200
O	-0.02759800	-1.40214000	-0.10386900
H	0.00301100	-1.55849600	0.85580600
H	-0.89387500	-0.17615000	-0.07327200
O	1.57493700	0.66785700	0.00233000
H	0.79384000	1.24179600	0.06034800
H	1.08622400	-0.22702900	-0.09025800

[OH(H₂O)₃]⁻:

E: -305.4088518

G293: -305.3479588

G243: -305.3423068

O	0.01374400	0.03892300	1.45233700
H	0.03989300	0.07279500	2.41898900
O	0.22015000	-1.65923500	-0.49071000
H	0.09994600	-1.24609600	0.42582800
H	0.81114200	-0.96568400	-0.84941100
O	1.31389200	1.00137800	-0.56167700
H	1.03802400	0.71686000	0.37267100
H	0.41006500	1.16522300	-0.89985700
O	-1.55050000	0.61382400	-0.52737600
H	-1.24153200	-0.25967600	-0.84356900
H	-1.13582500	0.55745600	0.39476700