Investigation of Rhodium Catalyzed Hydroboration with NHC-Boranes: Role of the Alkene Coordination and Origin of the Enantioselectivity

SUPPORTING INFORMATION

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## Summary

1- Experimental procedures

NHC-borane **3** (0.109 mmol, 1 equiv), [Rh(nbd)$_2$]BF$_4$ (0.109 mmol, 1 equiv) and (*S*)-Binap (0.109 mmol, 1 equiv) were added in 10 mL Schlenk flask under argon and dissolved in dry and degas deuterated dichloromethane (0.87 mL) at room temperature.

¹H NMR (400 MHz, CD$_2$Cl$_2$)

¹¹B NMR (128 MHz, CD$_2$Cl$_2$)

Reaction scheme showing Me–N/N–Me imidazole with BH₃ (3 equiv) reacting under Rh(nbd)₂ BF₄ (1 equiv), (S)-BINAP (1 equiv), DCM-d₂, rt, t.
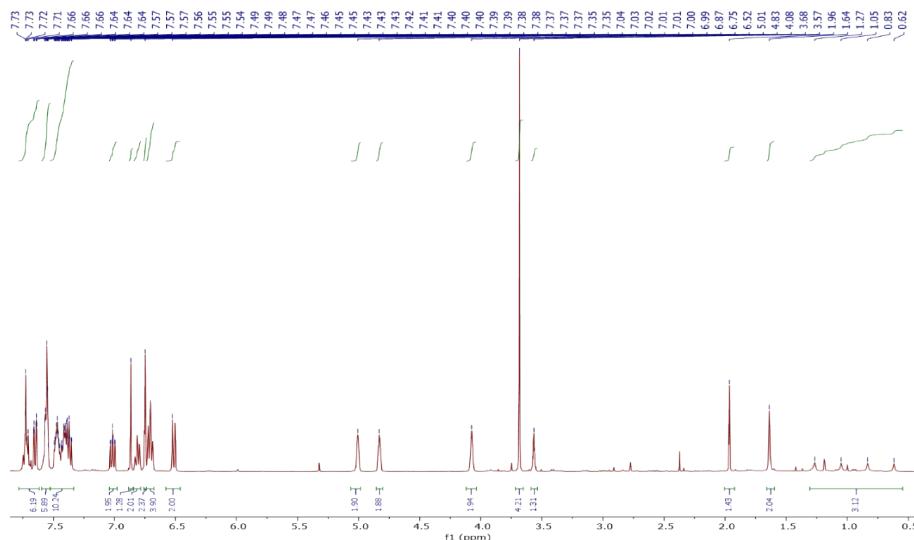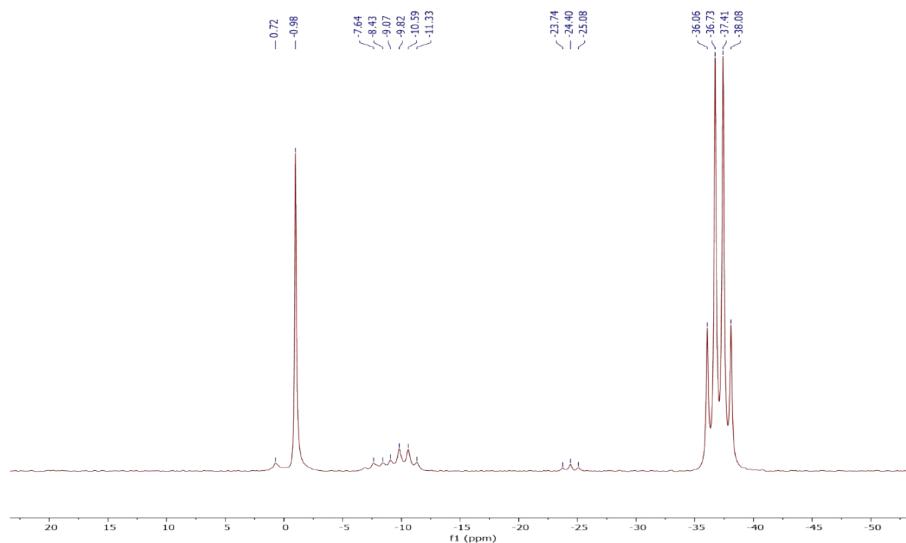
NHC-borane **3** (0.109 mmol, 3 equiv), [Rh(nbd)$_2$]BF$_4$ (0.0363 mmol, 1 equiv) and (S)-Binap (0.0363 mmol, 1 equiv) were added in 10 mL Schlenk flask under argon and dissolved in dry and degas deuterated dichloromethane (0.87 mL) at room temperature.

^{1}H NMR (400 MHz, CD$_2$Cl$_2$)

^{11}B NMR (128 MHz, CD$_2$Cl$_2$)

Reaction scheme: Me–N···N–Me imidazole with BH$_3$, 3 equiv → Rh(nbd)$_2$ BF$_4$ (1 equiv), DCM-d$_2$, rt, t
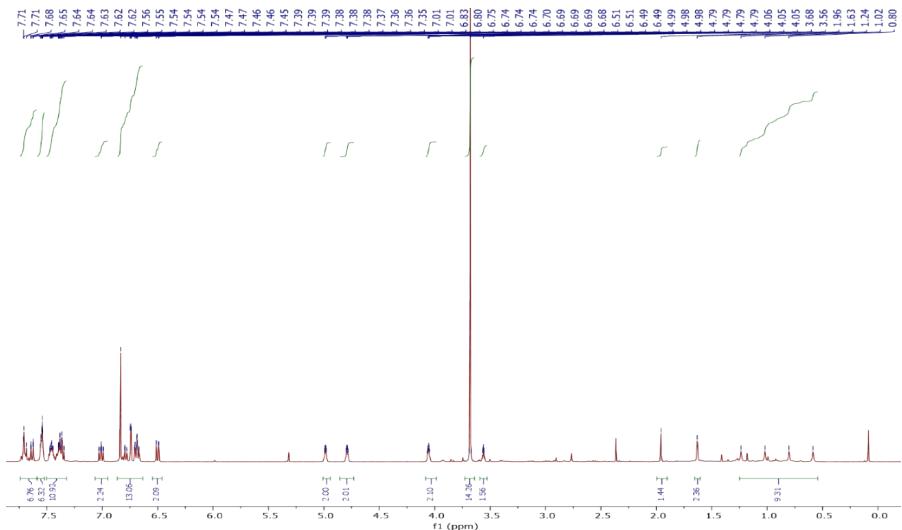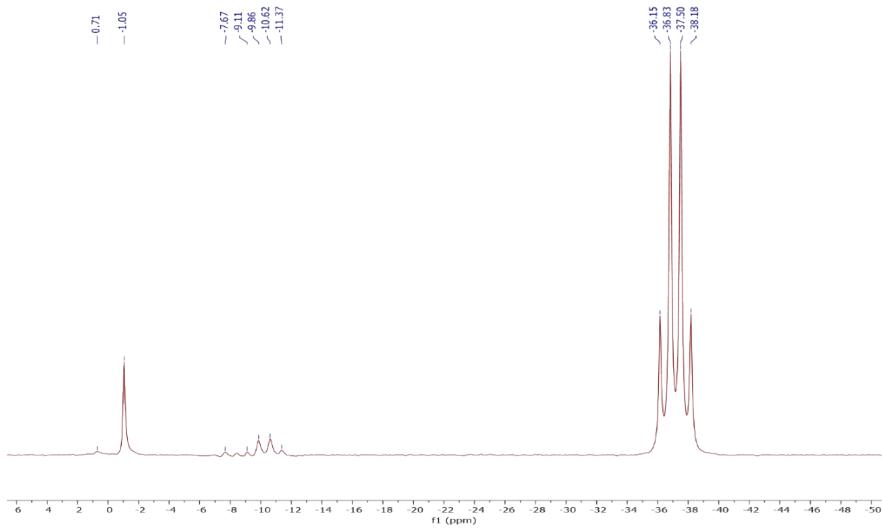
NHC-borane **3** (0.109 mmol, 3 equiv) and [Rh(nbd)$_2$]BF$_4$ (0.636 mmol, 1 equiv) were added in 10 mL

Schlenk flask under argon and dissolved in dry and degas deuterated dichloromethane (0.87 mL) at room

temperature.

^{1}H NMR (400 MHz, CD$_2$Cl$_2$)
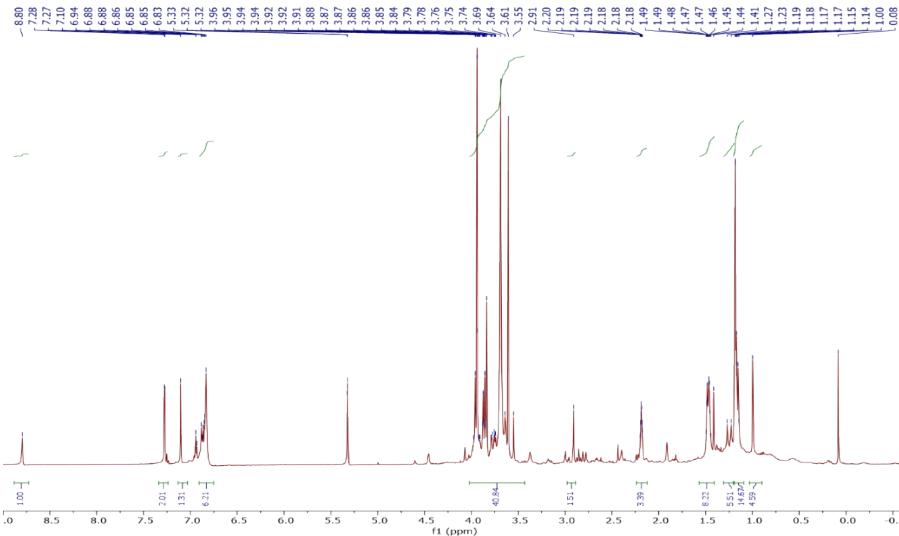
^{11}B NMR (128 MHz, CD$_2$Cl$_2$)

Rh(nbd)$_2$ BF$_4$ (1 equiv)
+
(S)-Binap

→ **DCM-d$_2$, rt**
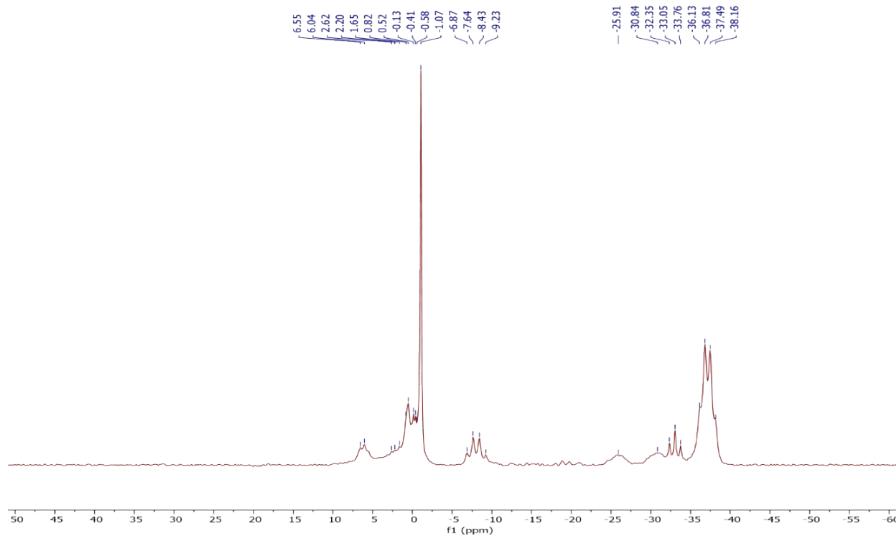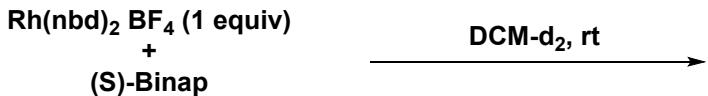
[Rh(nbd)$_2$]BF$_4$ (0.109 mmol, 1 equiv) and (*S*)-Binap (0.109 mmol, 1 equiv) were added in 10 mL Schlenk flask under argon and dissolved dry and degas deuterated dichloromethane (0.87 mL) at room temperature.

^{1}H NMR (400 MHz, CD$_2$Cl$_2$)
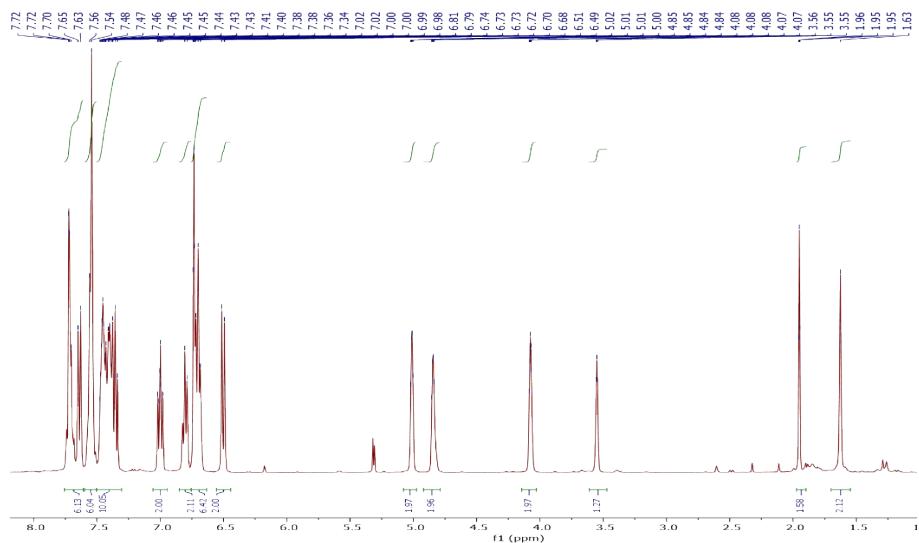
2- Comparison between computational methods

The RPA method includes dispersion effects in a non-empirical way and it does accurately take into account the interaction between the bulky ligand and the substrate, which is crucial for the enantioselectivity in our case. It is important, however, that this method reproduces correctly energies of the transition states. We cannot afford to do accurate CCSD(T) calculations on the real system. We have performed some CCSD(T) calculations (def2-QZVP basis set) on transition states for the hydride formation with a Wilkinson-type catalyst and H$_2$ or BH$_3$-NH$_3$ (Scheme S1).

Barrier (kcal/mol)

	CCSD(T)	RPA
H₃P–Rh(Cl)(H)(H) → H₃P–Rh(Cl)–H(H)	4.3	5.7
H₃P–Rh(Cl)(H)(H–BH·NH₃) → H₃P–Rh(Cl)–H(BH₂-NH₃)	11.1	12.6

$H_3P,\ Rh,\ Cl,\ H$ structures
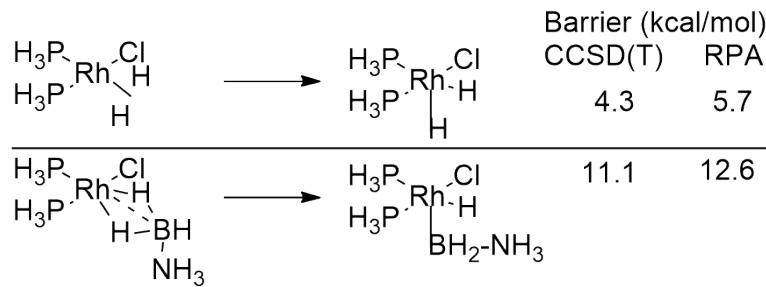
Scheme S1. Hydride formation with a Wilkinson-type catalyst.

The RPA calculations underestimate the energy barrier (electronic energy) by only 1.5 kcal/mol. The fact that this underestimation is small and systematic in the two cases, suggests that the error is the same for the pro-R and pro-S paths and it does not affect the comparison.

As DFT calculations were already employed for mechanistic studies of this kind, the comparison with several DFT functionals and B2PLYP allows us to check that there is not a major bias in the use of RPA for the other steps.

Structures discussed in the main article are optimized at the PBE-D3 level by using a def2-SVP basis set. Energies are obtained as single point calculations at the RPA (Random-Phase-Approximation) level (PBE functional) with a def2-QZVP basis set. Since RPA calculations are not routinely used for computations of mechanistic profiles yet, some preliminary calculations have been performed to check for accuracy. Two sets of calculations have been performed: a) the reaction profile has been computed for a model system: the (S)-MeO-xylyl-BIPHEP ligand was replaced by a simpler ligand L (the 4 aryl groups on the P atoms were replaced by H atoms) and the methyl group on the NHC was replaced by a hydrogen atom; b) the real system has been computed at the B2PLYP (basis set def2-TZVP) method as well (see the article for labels).

2.1. Model system

Table S1. Electronic energies (relative to the isolated [LRhNBD]$^+$ and the modified **1** systems, kcal/mol) for the hydroboration reaction in the model system. Energies barriers are also reported. Labels as in the article.

	BP86	PBE	BP86-D3	PBE-D3	PBE0	B3LYP	M06	B2PLYP	RPA
II	-3.95	-4.32	-6.64	-5.70	-3.83	-2.82	-4.6	-2.98	-3.95
Ts$_{II\text{-}III}$	8.42	8.47	4.94	6.60	10.60	10.95	9.4	8.92	7.61
III	6.50	6.27	1.25	3.46	8.43	9.48	8.0	5.23	3.29
Ts$_{III\text{-}IV}$	9.19	8.72	4.20	6.09	10.30	12.86	10.8	8.45	6.51
IV	4.33	3.80	-0.69	1.13	4.50	6.61	3.7	3.11	1.50
Ts$_{IV\text{-}VI}$	15.47	15.28	14.17	14.47	15.48	16.96	14.2	17.36	15.59
VI	-12.20	-12.12	-11.09	-11.59	-15.13	-14.03	-12.8	-10.43	-8.15
Computed barriers									
II to III	12.37	12.79	11.58	12.3	14.43	13.77	14.00	11.9	11.56
III to IV	2.69	2.45	2.95	2.63	1.87	3.38	1.87	3.22	3.22
IV to VI	11.14	14.86	14.86	13.34	10.98	10.35	10.98	14.25	14.09
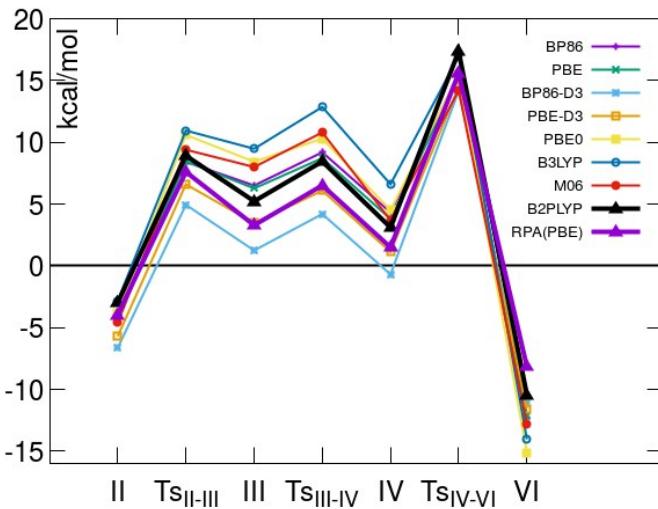
Figure S1 Energetic profiles for the reaction in the model systems, *via* the [Rh]-H migratory insertion mechanism. Comparison of several methods. See the article for labels (Figure 1). Energies are relative to isolated [LRhNBD]⁺ and the modified **1** systems.

In the model system we computed only the mechanism through the [Rh]-H migratory insertion step. For DFT calculations, structures were re-optimized at each functional (basis set: def2-SVP), for B2PLYP (def2-TZVP) and RPA (def2-QZVP), single point energy calculations are performed on the PBE-D3 structures. Electronic energies, reported in Table S1 and depicted in Figure S.1 are related to the isolated [LRhNBD]⁺ and the modified **1** systems. The conformational change from intermediates **C** to **D** is not necessary. The transition state **Ts$_{CE}$** corresponds to the reductive elimination.

The main result here is that all methods perform very similarly, since the curves are almost parallel. The methods that contain the semi-empirical dispersion factors are the lowest curves. This might be due to an overestimation of the stabilization of intermediate **A**, which is obtained by substitution of the NBD by the substrate. Table S1 reports as well the barriers between the intermediates. Interestingly, the RPA and the B2PLYP methods provide the same barrier heights. Furthermore, we notice that for this model system, where the L ligand has not the same steric hindrance than the real one, the highest energy is computed for the transition state responsible for the reductive elimination. The methods that do not contain dispersion corrections, tend to slightly underestimate the barrier of the reductive elimination step, thus overestimating the steric decompression that this event causes.
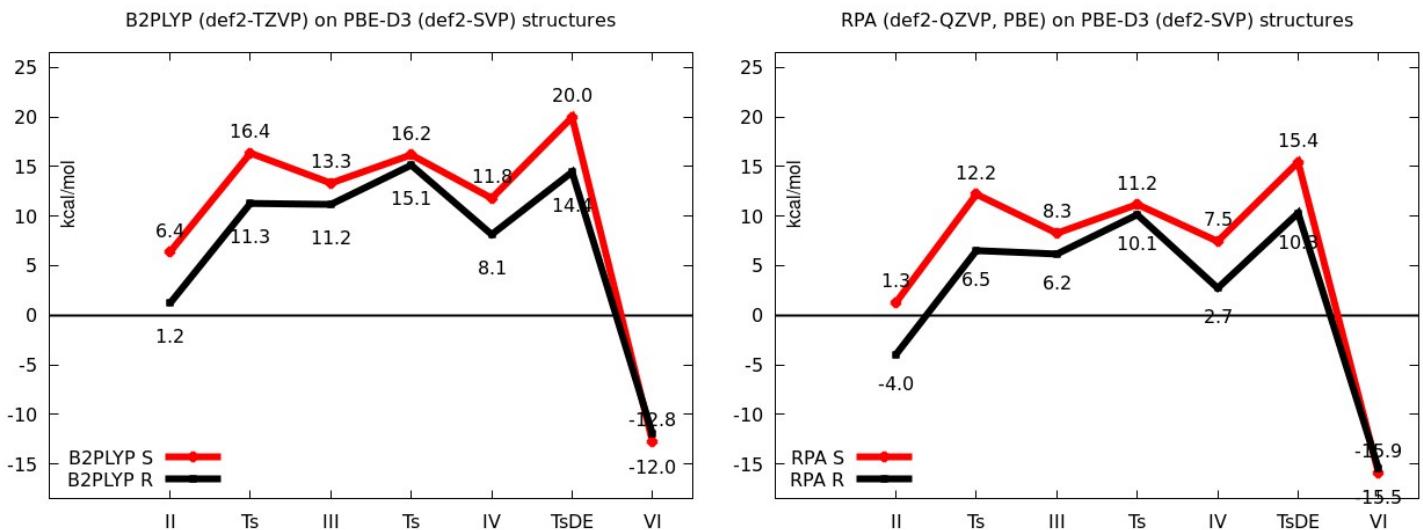
Fig. S2 Comparison between the computed energetic profiles at the B2PLYP and RPA methods for the real system, *via* the [Rh]-H migratory insertion mechanism.). Energies are relative to isolated [LRhNBD]$^+$ and the modified **1** systems.

2.2. Real system

We compare now the B2PLYP and RPA pro-*R* and pro-*S* computed energetic pathway for the real system, *via* the [Rh]-H migratory insertion step (structures are obtained at the PBE-D3 level, by employing the def2-SVP basis set. Single point calculations at the B2PLYP and RPA levels are performed with a def2-TZVP basis set, Figure S2). Here again we notice that the RPA and the B2PLYP curves are parallel. The deviation from the two methods is due to the position of our zero for the energy (isolated [LRhNBD]$^+$ and substrate), which causes (only) a shift between the two methods.

3. Mechanism through the [Rh]-B migratory step

Besides the mechanism *via* the [Rh]-H migratory insertion, another pathway could be invoked, *via* a [Rh]-B migratory insertion step, instead of through the Rh-H migratory insertion into the alkene moiety (Scheme S2). From **I**, after a first transition state, a hydride structure **III_B** results. The B-C bond is then formed (**IV_B**) and the reductive elimination leads to the final product **VI**, coordinated to the metal.
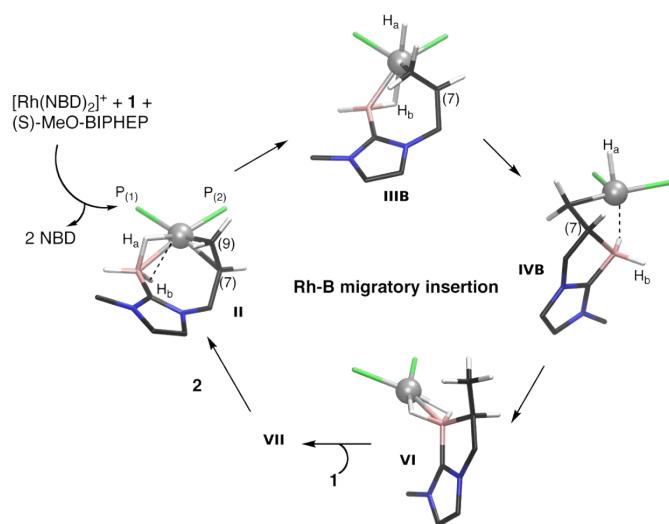
Scheme S2. Schematic representation of the Rh catalyzed hydroboration reaction *via* a [Rh]-B migratory insertion mechanism.

This mechanism is computed to be possible for the pro-*S* profile, as shown in Figure S3. The pro-*S* [Rh]-H vs. [Rh]-B migration insertion mechanism profiles are energetically almost equivalent and they possibly coexist (Figure S3). In Figure S4, the structures of **III_S**, **III_BS**, **III_R** and **III_BR** are compared. In the **III_BS** intermediate, the H_a-Rh bond is orthogonal to the P(1)-P(2)-Rh plane. The -BH_2 fragment also moves from this plane, so that a further interaction is formed between H_b and the metal center that contributes to stabilize the complex. A structure results, where the H_a, the Rh and the H_b atoms are collinear.
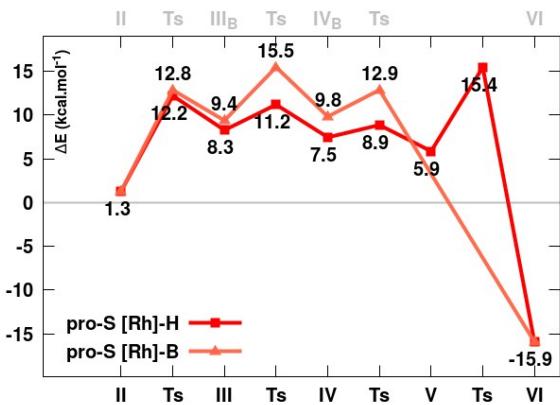
Figure S3. Comparison between the pro-*S* mechanisms, *via* either the [Rh]–H migratory insertion mechanism (red) or the [Rh]–B migratory insertion mechanism (pink). Labels are as in Figure 1 (main article, [Rh]–H migratory insertion mechanism, on the x axis) and Scheme S2 ([Rh]–B migratory insertion mechanism, on the opposite x axis). Energies (electronic energies, ZPE corrected) are related to the isolated [(L)Rh-NBD]$^+$ (L=*S*-MeO-xylyl-BIPHEP) complex and substrate **1**.
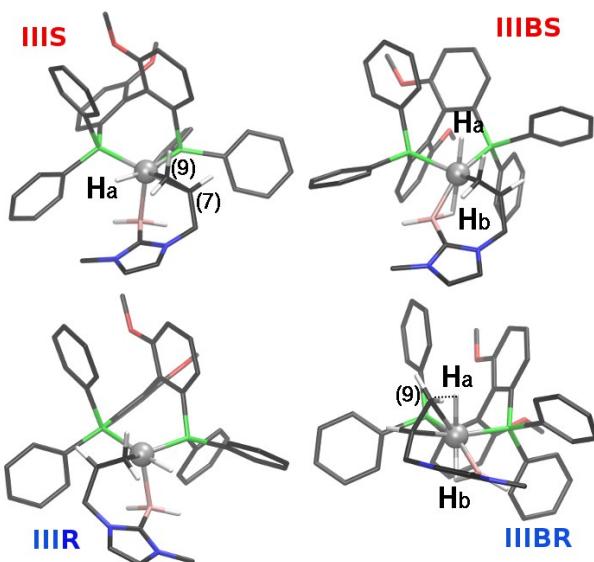
Figure S4. Computed structures of intermediates **III$_S$**, **III$_{BS}$**, **III$_R$** and **III$_{BR}$** (PBE-D3/def2-SVP level).

We could not optimize structures for the pro-*R* [Rh]-B migratory insertion mechanism. Indeed, any attempt to obtain a valid **III$_{BR}$** intermediate lead us to either **III$_R$** or to the structure presented in Figure S4. The latter is higher in energy than all the transition states of the pro-*R* [Rh]-H migratory insertion mechanism; furthermore, the hydride H$_a$ is very close to the C(9) atom (121 pm), which would indeed favor the [Rh]-H than the [Rh]-B migratory insertion.

4. Substitution of the *R* product

4.1. Alkene approach

We report here (Figure S5) results obtained for the substitution of the final R product by prior coordination of the alkene moiety of the new substrate, which is intrinsically enantioselective and is possible for the pro-S approach, while the pro-R implies a large approaching barrier (18.7 kcal/mol). The first transition state corresponds to the approach of the alkene moiety to the metal center. Some conformational changes take place, for which the transition states have not been searched. The second transition state determines the final expulsion of the product.
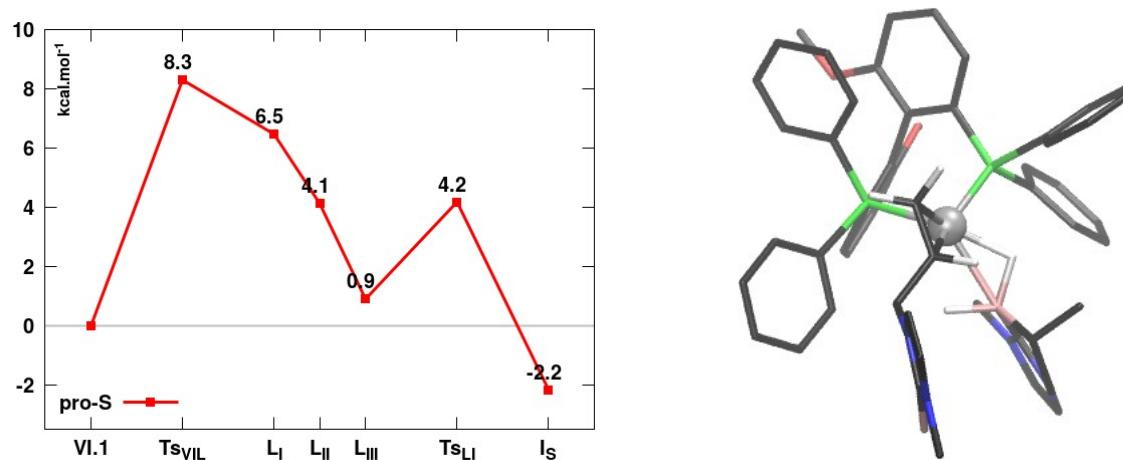
Fig. S5 Computed pathway (electronic energies corrected by the ZPE) for the substitution of the final R product by a new substrate, pro-*S* approach. The $\mathbf{L_I}$ structure is also depicted.

4.2. BH$_3$ Approach

The last step of the BH$_3$ approach is the removal of the product and the coordination of the alkene moiety. The structures of the corresponding transition states are shown in the main article. The **TS$_{VII-IS}$** has a closer structure to the intermediate **VIIc** concerning the orientation of the NHC group, while in **TS$_{VII-IR}$**, the NHC fragment needs to undergo a rotation about the C-B bond to reach the best conformation for the alkene approach to the metal center. This is revealed by the values of the Rh-B-C-N dihedral angles, which are of 78^0 and of 63^0 for **VIIc** and **TS$_{VII-IS}$**, respectively, while its value is of 3.5^0 for **TS$_{VII-IR}$**.

5. Energies and xyz coordinates

Energies. Total energies and ZPE (in a.u.) for computed structures at the optimizing level (def2-TZVP/PBE-D3) and at the def2-QZVP/RPA(PBE) level are reported. Cartesian coordinates of all intermediates and transition states at the optimizing level follow. See the article for labels, R for pro-R structures, S for pro-S structures.

	PBE-D3 (a.u.)	ZPE (a.u.)	Chemical Potential (kJ/mol)	RPA (a.u.)
0	-2817.819224300	0.7671902	1762.09	-2820.1290840594
Ts$_{0\text{-}IR}$	-2817.809595906	0.7667683	1763.22	-2820.1179360517
Ts$_{0\text{-}IIR}$	-2817.816094756	0.7671041	1764.29	-2820.1267263527
I$_R$	-2817.840231936	0.7691105	1781.02	-2820.1502164133
Ts$_{I\_IIR}$	-2817.826371612	0.7690246	1782.34	-2820.1358488962
II$_R$	-2817.834022961	0.7686395	1775.37	-2820.1430670865
Ts$_{II\_IIIR}$	-2817.814902887	0.767174	1773.8	-2820.1244815121
III$_R$	-2817.814997231	0.7675123	1767.39	-2820.1254425507
Ts$_{III\_IVR}$	-2817.80776245	0.7659951	1769.3	-2820.1173665672
IV$_R$	-2817.822143244	0.7690815	1776.16	-2820.1324004661
Ts$_{IV\_VR}$	-2817.821604328	0.7685437	1776.08	-2820.130212813
V$_R$	-2817.828048253	0.7699276	1779.18	-2820.1388822925
Ts$_{V\_VIR}$	-2817.81167643	0.7682014	1772.5	-2820.1197375168
VI$_R$	-2817.853890877	0.7703957	1773.28	-2820.1631096595
III$_{BR}$	-2817.806229631	0.7672569	1775.48	-2820.1145148406
Ts$_{0\_IS}$	-2817.813326731	0.767274	1771.95	-2820.1229271136
Ts$_{0\_IIS}$	-2817.806689203	0.7669511	1765.14	-2820.1154432734
I$_S$	-2817.830160454	0.7686507	1778.67	-2820.1379558464
Ts$_{I\_IIS}$	-2817.81366756	0.7677426	1773.05	-2820.1207952961
II$_S$	-2817.825872054	0.7688716	1777.86	-2820.1351529934
Ts$_{II\_IIIS}$	-2817.80662667	0.7662998	1769.67	-2820.1147686169
III$_S$	-2817.812577848	0.767413	1774.06	-2820.1213648723
Ts$_{III\_IVS}$	-2817.807631559	0.7659254	1771.86	-2820.1153692449
IV$_S$	-2817.816724416	0.7694001	1778.04	-2820.1251895569
Ts$_{IV\_VS}$	-2817.815582085	0.7695491	1782.04	-2820.1231045517

V_S	-2817.818912203	0.7694912	1773.76	-2820.1277841884
Ts_{V_VIS}	-2817.803423396	0.7685371	1771.49	-2820.1116805098
VI_S	-2817.854979644	0.7702485	1769.98	-2820.1637318762
$VIR.1$	-3226.384437318	0.9592599	2216.68	-3229.3490145167
$VIIa$	-3226.385457261	0.9587476	2223.54	-3229.3480557458
$VIIb$	-3226.386176385	0.9605426	2230.07	-3229.353969072
$VIIc$	-3226.392656199	0.9602854	2234.06	-3229.3613724941
Ts_{VII_IS}	-3226.367425658	0.95909	2224.29	-3229.3324844031
Ts_{VII_IR}	-3226.365402536	0.9581649	2216.17	-3229.3287989484

Xyz Coordinates

0.xyz
98
Energy = -2817.819224300

Rh	-1.5938724	-0.1452963	-0.3693164
P	-0.3316567	-1.4524822	0.8909634
P	0.1853009	0.6200425	-1.4343583
C	-0.4314179	1.5149098	-2.9203558
C	-0.0511416	2.8297486	-3.2284605
C	-1.4013190	0.8823239	-3.7208812
C	-0.6207370	3.4921907	-4.3193238
H	0.6851864	3.3480234	-2.6144082
C	-1.9547555	1.5402185	-4.8174836
H	-1.7378388	-0.1250777	-3.4661240
C	-1.5672496	2.8498384	-5.1183394
H	-0.3197757	4.5171395	-4.5421709
H	-2.6992569	1.0326793	-5.4328540
H	-2.0083083	3.3690405	-5.9706166
C	1.2972599	-0.7133910	-2.0302731
C	2.1158364	-1.3805097	-1.0962954
C	1.1997144	-1.1764687	-3.3509665
C	2.8028868	-2.5468797	-1.5138379
C	1.8968663	-2.3168477	-3.7406896
H	0.5858132	-0.6446576	-4.0759221
C	2.6853202	-3.0152293	-2.8286736
H	1.8222839	-2.6724347	-4.7695023
H	3.2118677	-3.9132150	-3.1469113
C	1.2947435	1.8310965	-0.6194204
C	2.5062549	2.2094784	-1.2205410
C	0.9147774	2.4183710	0.5946655
C	3.3132591	3.1748795	-0.6184473
H	2.8236925	1.7369875	-2.1520359
C	1.7285735	3.3775633	1.1998612
H	-0.0145522	2.0924312	1.0695754
C	2.9259565	3.7609350	0.5907327
H	4.2509814	3.4684721	-1.0936219
H	1.4318001	3.8202713	2.1521933
H	3.5624402	4.5117898	1.0617490
C	-0.1459389	-3.1691584	0.2863590
C	0.7596995	-4.0529918	0.8951481
C	-0.9154182	-3.6031384	-0.8026605
C	0.8821962	-5.3594106	0.4216808
H	1.3809233	-3.7139930	1.7261274
C	-0.7809030	-4.9074902	-1.2794381
H	-1.6025467	-2.8996165	-1.2799088
C	0.1159396	-5.7865938	-0.6670495
H	1.5842591	-6.0443477	0.9004661
H	-1.3747053	-5.2369530	-2.1333894
H	0.2194144	-6.8073221	-1.0391640
C	-1.2008009	-1.5756612	2.5066901
C	-1.5184545	-0.3819968	3.1815651
C	-1.6006890	-2.7991577	3.0613412
C	-2.1872473	-0.4167029	4.4041663
H	-1.2384366	0.5768199	2.7386602
C	-2.2926359	-2.8284659	4.2761304
H	-1.3738895	-3.7328146	2.5454319
C	-2.5785166	-1.6421598	4.9542158
H	-2.4083390	0.5162221	4.9264144
H	-2.6015753	-3.7869351	4.6962751
H	-3.1065893	-1.6711066	5.9086957
C	1.3857993	-0.9615161	1.3236830
C	1.7115183	-0.5610198	2.6290887
C	2.3493540	-0.8966708	0.2976954
C	2.9861425	-0.0789196	2.9137282
H	0.9754164	-0.6347830	3.4270726
C	3.6313089	-0.3787603	0.6073059
C	3.9454690	0.0288908	1.9098059
H	3.2369258	0.2224320	3.9320137
H	4.9321975	0.4237261	2.1452565
O	4.4934429	-0.2908475	-0.4396356
O	3.5500008	-3.1586835	-0.5573091
C	5.8047040	0.2166264	-0.1931954
H	6.3167886	0.1938072	-1.1612502
H	5.7686043	1.2537886	0.1790304
H	6.3512021	-0.4149379	0.5257454
C	4.2463185	-4.3544789	-0.9078101
H	4.7657599	-4.6710791	0.0032689
H	3.5461827	-5.1447842	-1.2244589
H	4.9846665	-4.1710451	-1.7051413
C	-4.3774478	2.3900564	2.7526196
C	-3.7439119	3.3334448	1.9974966
C	-3.8864965	1.4544676	0.7654576
N	-4.4646970	1.2488501	1.9767282
H	-4.7807520	2.4393251	3.7567897
H	-3.4808964	4.3608535	2.2158381
N	-3.4625146	2.7466797	0.7759941
C	-2.7345185	3.3884034	-0.3383092
H	-3.2296830	3.0738762	-1.2690346
H	-1.7140198	2.9789168	-0.3600272
C	-2.7087955	4.8812306	-0.2360115
H	-3.6752230	5.3947198	-0.2736985
C	-1.5751594	5.5826873	-0.1605129
H	-0.6010780	5.0871997	-0.1295529
H	-1.5804038	6.6730418	-0.1409727
C	-5.0732739	-0.0147663	2.3764802
B	-3.7366972	0.3541187	-0.3704202
H	-4.7900189	0.0462125	-0.8849731
H	-2.9422673	0.7313077	-1.3055930
H	-3.2675521	-0.7530652	0.1320764
H	-4.3044286	-0.7942913	2.4545326
H	-5.5541202	0.1166944	3.3511384
H	-5.8225263	-0.3146754	1.6333930

IR.xyz
98
Energy = -2817.840231936

Rh	1.4572895	0.2791632	-0.5586963
P	-0.1964442	1.6867258	-0.0076347
P	-0.0379773	-1.4874953	-0.5390375
C	0.6420543	-2.7014145	-1.7384680
C	0.9133081	-4.0330412	-1.3980448
C	0.9855621	-2.2422775	-3.0233357
C	1.5046664	-4.8914151	-2.3295020
H	0.6733174	-4.4040813	-0.4017302
C	1.5611571	-3.1045729	-3.9543901
H	0.8043303	-1.1980291	-3.2872052
C	1.8245287	-4.4337442	-3.6080131
H	1.7140376	-5.9251860	-2.0497315
H	1.8109961	-2.7377323	-4.9514428
H	2.2821973	-5.1081503	-4.3334031
C	-1.7486172	-1.1437076	-1.1201494
C	-2.5896955	-0.3686387	-0.2981681
C	-2.1905803	-1.5776496	-2.3788692
C	-3.8751157	-0.0191725	-0.7796603
C	-3.4651286	-1.2353756	-2.8240907
H	-1.5481364	-2.1952629	-3.0040984
C	-4.3082847	-0.4519926	-2.0391230
H	-3.8090934	-1.5832949	-3.7994906
H	-5.2961386	-0.1833935	-2.4089680
C	-0.3583710	-2.4582676	0.9892436
C	-1.3440461	-3.4601061	0.9803677
C	0.3494353	-2.2034059	2.1701410
C	-1.5978907	-4.2064317	2.1307943
H	-1.9238325	-3.6470195	0.0746073
C	0.0828606	-2.9419158	3.3240435
H	1.0996065	-1.4138444	2.1869943
C	-0.8860976	-3.9475893	3.3058637
H	-2.3611166	-4.9863466	2.1114290
H	0.6307258	-2.7263810	4.2429357
H	-1.0897816	-4.5282459	4.2073165
C	-1.4438349	2.2791534	-1.2153707
C	-2.4922301	3.1019889	-0.7690321
C	-1.3792222	1.9202411	-2.5678038
C	-3.4403985	3.5802211	-1.6729062
H	-2.5750638	3.3569042	0.2891168
C	-2.3369940	2.3897697	-3.4666044
H	-0.5939227	1.2424649	-2.9032844
C	-3.3633512	3.2270215	-3.0231468
H	-4.2465979	4.2248568	-1.3186519
H	-2.2862707	2.0926066	-4.5151003
H	-4.1083361	3.5990103	-3.7284630
C	0.5886603	3.2225875	0.6393381
C	1.6086316	3.0940612	1.6021919
C	0.2884956	4.4989797	0.1422667
C	2.2770875	4.2179447	2.0840630
H	1.8937737	2.1012330	1.9562865
C	0.9727362	5.6223739	0.6158785
H	-0.4779935	4.6245731	-0.6221767
C	1.9592102	5.4879302	1.5926254
H	3.0557623	4.1011758	2.8398042
H	0.7284625	6.6074122	0.2151591
H	2.4866993	6.3676251	1.9645065
C	-1.2284085	1.0243488	1.3668020
C	-0.9733734	1.4081016	2.6925906
C	-2.2133982	0.0554710	1.0822296
C	-1.6835822	0.8231666	3.7374453
H	-0.2378483	2.1790956	2.9118058
C	-2.9137284	-0.5336894	2.1652671
C	-2.6448117	-0.1523845	3.4856656
H	-1.4867184	1.1322044	4.7652238
H	-3.1823800	-0.6085149	4.3149988
O	-3.8247164	-1.4809366	1.8253107
O	-4.6170501	0.7623830	0.0482404
C	-4.5494258	-2.1286373	2.8703295
H	-5.2103407	-2.8448120	2.3700207
H	-3.8703929	-2.6698751	3.5492348
H	-5.1558910	-1.4094792	3.4443577
C	-5.9248920	1.1427840	-0.3771410
H	-6.3333214	1.7547641	0.4344762
H	-5.8853280	1.7402157	-1.3028711
H	-6.5687137	0.2619048	-0.5321698
C	6.7481622	0.1799625	0.8938857
C	6.3875516	0.9659275	-0.1609175
C	4.6376001	-0.3648033	0.3242131
N	5.6641212	-0.6355497	1.1728460
H	7.6704530	0.1312052	1.4603274
H	6.9403846	1.7251469	-0.7013777
N	5.0920364	0.6192760	-0.4914919
C	4.3126163	1.1540843	-1.6179376
H	4.1792077	0.3485710	-2.3565309
H	4.9454801	1.9282457	-2.0802847
C	2.9768111	1.7330472	-1.2240515
H	3.0331004	2.5841742	-0.5391822
C	1.9025799	1.6827542	-2.1444237
H	2.0136193	1.1222666	-3.0789195
H	1.2237661	2.5333781	-2.2201086
C	5.6138627	-1.6050045	2.2606885
B	3.1922690	-0.9951729	0.2867569
H	3.1381118	-2.1408900	0.6675854
H	2.4231503	-0.2674350	1.0095989
H	2.7866676	-0.9832576	-0.9345122
H	4.8076233	-2.3172398	2.0585604
H	6.5706020	-2.1375846	2.3184820
H	5.4195158	-1.0980551	3.2157968

IIR.xyz
98
Energy = -2817.834022961
Rh -1.3790477   0.6106062 -0.0366178
H   -3.4229413 -1.5247073 -1.3304781
B   -3.3310921 -0.3750701 -0.9738112
H   -2.7315526 -0.4813373   0.1810673
H   -2.7114717   0.3452133 -1.7671916
C   -4.6912251   0.2633903 -0.5064283
C   -6.1600609   1.7694918   0.2978193
C   -6.7529552   0.5413458   0.3528177
H   -6.5292923   2.7486783   0.5782589
H   -7.7379151   0.2458509   0.6937530
N   -4.8970632   1.5766626 -0.2298991
N   -5.8371673 -0.3692190 -0.1432273
C   -3.9046559   2.6195025 -0.4881017
H   -3.7114473   2.6516728 -1.5715963
H   -4.3831401   3.5751526 -0.2191364
C   -2.6014137   2.4855919   0.2671979
H   -1.9566715   3.3401980   0.0558448
C   -2.3953242   1.8000107   1.4724199
H   -3.1898907   1.1849167   1.9044096
H   -1.6711905   2.1852941   2.1902702
C   -6.0325423 -1.8157150 -0.2050027
H   -5.8444137 -2.1752032 -1.2228167
H   -5.3404435 -2.3197703   0.4828599
H   -7.0657509 -2.0410751   0.0795043
P   0.5967201   1.7386950 -0.0753291
P   -0.2852243 -1.4190567   0.1298711
C   1.8183143   0.9160349 -1.1919707
C   2.4858854 -0.2448510 -0.7514358
C   2.0095516   1.3815058 -2.5028167
C   3.3270804 -0.9323967 -1.6620741
C   2.8443446   0.6917843 -3.3775020
H   1.5251325   2.2946031 -2.8409615
C   3.4981108 -0.4686477 -2.9717661
H   2.9903944   1.0652328 -4.3922769
H   4.1406266 -1.0008646 -3.6708167
C   1.2490701 -1.4226172   1.1431134
C   2.3953143 -0.7792284   0.6383313
C   1.2581484 -1.9748809   2.4334998
C   3.5420428 -0.6852136   1.4644651
C   2.4005354 -1.8789734   3.2238622
H   0.3809832 -2.4925569   2.8171331
C   3.5403653 -1.2299778   2.7543877
H   2.4051548 -2.3172899   4.2231690
H   4.4201261 -1.1539945   3.3908719
C   0.2028764 -2.2989494 -1.4005001
C   1.0305081 -3.4325290 -1.3439303
C   -0.2635357 -1.8442985 -2.6411891
C   1.3757383 -4.1042968 -2.5164580
H   1.4161183 -3.7797218 -0.3836909
C   0.0943206 -2.5121156 -3.8132027
H   -0.9051307 -0.9625278 -2.6849375
C   0.9121538 -3.6429483 -3.7523764
H   2.0135376 -4.9885748 -2.4651617
H   -0.2653184 -2.1469402 -4.7764284
H   1.1890027 -4.1666064 -4.6690098
C   -1.4214269 -2.5854765   0.9936710
C   -2.0328998 -2.1594312   2.1871229
C   -1.7855640 -3.8235586   0.4504191
C   -2.9720115 -2.9631590   2.8307442
H   -1.7791263 -1.1812812   2.6019227
C   -2.7397622 -4.6218365   1.0897659
H   -1.3392530 -4.1650435 -0.4835088
C   -3.3325489 -4.1978995   2.2795018
H   -3.4276269 -2.6239882   3.7628479
H   -3.0169541 -5.5819242   0.6511184
H   -4.0717135 -4.8263964   2.7790890
C   0.3460145   3.4045199 -0.8255968
C   0.7699854   4.5967245 -0.2237614
C   -0.4035172   3.4769963 -2.0165628
C   0.4737361   5.8310702 -0.8116846
H   1.3252610   4.5717374   0.7136822
C   -0.6848735   4.7067609 -2.6077138
H   -0.7872914   2.5588628 -2.4685973
C   -0.2438610   5.8903224 -2.0059758
H   0.8086198   6.7498402 -0.3275413
H   -1.2551772   4.7430089 -3.5375808
H   -0.4680353   6.8546699 -2.4644241
C   1.5570989   2.0542387   1.4527163
C   1.0386430   1.6863473   2.7011663
C   2.8241338   2.6578874   1.3820644
C   1.7636325   1.9368910   3.8666825
H   0.0836473   1.1612368   2.7462284
C   3.5417531   2.9159492   2.5496001
H   3.2558203   2.9103892   0.4118398
C   3.0110937   2.5605971   3.7934983
H   1.3576032   1.6346324   4.8331828
H   4.5235413   3.3886164   2.4867987
H   3.5750682   2.7633117   4.7055074
O   3.9196660 -2.0543587 -1.1760500
O   4.6003443 -0.0279653   0.9216515
C   4.7842350 -2.7895414 -2.0416104
H   5.1466765 -3.6353277 -1.4471197
H   4.2397889 -3.1671029 -2.9225719
H   5.6402925 -2.1771656 -2.3681939
C   5.7916429   0.0881830   1.6987845
H   6.2078567 -0.9019715   1.9456046
H   6.5020578   0.6360829   1.0701458
H   5.6091513   0.6552717   2.6263514

IIIR.xyz
98
Energy = -2817.814997231

Rh	-1.3758120	0.4220249	0.6346224
H	-2.2991446	0.8703910	-1.7969673
H	-2.5633329	-0.4889008	1.1022825
B	-2.8858701	0.1773150	-0.9888745
H	-3.0578438	-0.9732220	-1.3192397
C	-6.3245719	1.3274854	0.1213883
C	-5.5877159	2.4595319	0.3242477
H	-7.3778906	1.1309196	0.2819201
H	-5.8725672	3.4303240	0.7121927
C	-4.2037238	0.8790048	-0.4988227
N	-4.2977756	2.1679950	-0.0687787
N	-5.4592766	0.3685293	-0.3731698
C	-2.1692721	2.4817065	1.1437303
C	-2.5403846	1.5376921	2.1023960
H	-3.5704421	1.1907687	2.1800754
H	-1.9584689	1.4420225	3.0232553
H	-1.3205329	3.1403089	1.3369671
P	-0.5130716	-1.6580491	0.2423198
P	0.5851947	1.6074462	-0.1660288
C	0.9917249	-1.6132690	1.3074882
C	2.1480902	-0.9332757	0.8623313
C	0.9142431	-2.0898245	2.6267891
C	3.2025585	-0.7267501	1.7880026
C	1.9693755	-1.8831973	3.5105564
H	0.0345399	-2.6377843	2.9595088
C	3.1085242	-1.1916208	3.1058477
H	1.9048493	-2.2651914	4.5306565
H	3.9210384	-1.0269094	3.8113132
C	1.8459454	0.6753039	-1.1219763
C	2.2405391	1.0871019	-2.4041375
C	2.3986378	-0.4839947	-0.5439508
C	3.1671814	0.3390167	-3.1239643
H	1.8347862	1.9984848	-2.8385099
C	3.3394852	-1.2283192	-1.2983681
C	3.7122658	-0.8238190	-2.5853273
H	3.4707421	0.6648294	-4.1200750
H	4.4281032	-1.4042693	-3.1644425
C	-3.1247105	3.0227057	0.1005096
H	-3.4847755	4.0217005	0.3917782
H	-2.6195738	3.1265856	-0.8711896
C	-5.8391968	-0.9961437	-0.7260606
H	-5.9971597	-1.0842751	-1.8087893
H	-5.0407786	-1.6828950	-0.4248095
H	-6.7654683	-1.2504699	-0.1990918
C	0.0726524	-2.2725029	-1.3781981
C	0.9065397	-3.4032404	-1.4241137
C	-0.3295810	-1.6604623	-2.5716843
C	1.3201518	-3.9171187	-2.6522549
H	1.2447289	-3.8711865	-0.4979027
C	0.0989207	-2.1715918	-3.7980972
H	-0.9786992	-0.7858331	-2.5366882
C	0.9186940	-3.3011939	-3.8412908
H	1.9610134	-4.8001674	-2.6801944
H	-0.2114053	-1.6848502	-4.7240241
H	1.2470239	-3.7019463	-4.8017001
C	-1.5823967	-3.0300480	0.8635755
C	-2.2714398	-2.8664341	2.0794433
C	-1.7842062	-4.2105788	0.1343931
C	-3.1076853	-3.8689776	2.5678233
H	-2.1654785	-1.9361124	2.6401769
C	-2.6395045	-5.2063548	0.6158802
H	-1.2886518	-4.3573053	-0.8241794
C	-3.2958409	-5.0448615	1.8354689
H	-3.6212777	-3.7268663	3.5202160
H	-2.7903441	-6.1125856	0.0270765
H	-3.9579056	-5.8262617	2.2118069
C	0.1420079	3.0476061	-1.2092518
C	0.2501251	4.3657672	-0.7375702
C	-0.4770699	2.8231709	-2.4537271
C	-0.2416454	5.4324816	-1.4945184
H	0.7250234	4.5649626	0.2240239
C	-0.9556098	3.8922374	-3.2117996
H	-0.5897057	1.8064782	-2.8312111
C	-0.8428265	5.2006620	-2.7331554
H	-0.1446665	6.4508203	-1.1143813
H	-1.4236800	3.6995771	-4.1785171
H	-1.2194311	6.0357916	-3.3255809
C	1.5977917	2.3079450	1.1968884
C	2.8023375	2.9766531	0.9229782
C	1.1974318	2.1375789	2.5286737
C	3.5726907	3.4895409	1.9655888
H	3.1408637	3.0866738	-0.1090824
C	1.9744632	2.6423496	3.5732831
H	0.2869578	1.5774397	2.7511636
C	3.1591306	3.3255103	3.2919543
H	4.5041886	4.0129705	1.7435197
H	1.6569104	2.4950429	4.6066333
H	3.7656764	3.7258425	4.1061095
O	4.2787667	-0.0536867	1.3030392
O	3.8231242	-2.3440394	-0.6888370
C	5.3709750	0.2047535	2.1848825
H	6.1070316	0.7536467	1.5874784
H	5.0564441	0.8278760	3.0376781
H	5.8215831	-0.7315093	2.5522073
C	4.7987564	-3.1210890	-1.3825573
H	5.0506041	-3.9481660	-0.7098722
H	4.3931607	-3.5248155	-2.3247763
H	5.7048179	-2.5306069	-1.5944015

IVR.xyz
98
Energy = -2817.822143244

Rh	-1.0698878	-0.8045117	1.0044425
H	-1.7773939	-1.1508419	-1.7239414
H	-1.5494330	-2.4697611	1.9772614
B	-2.1598960	-1.6163203	-0.6635198
H	-1.8371618	-2.7914176	-0.5298804
C	-5.8934421	-1.7346400	-1.2085742
C	-5.8890260	-1.1162241	0.0051476
H	-6.7135449	-2.0466894	-1.8443404
H	-6.7043210	-0.7641576	0.6253966
C	-3.7411579	-1.4822652	-0.5701229
N	-4.5639602	-0.9759952	0.3814541
N	-4.5705498	-1.9512501	-1.5455564
C	-2.7929492	-0.6276770	2.1238526
C	-2.5219099	-2.0795575	2.4547605
H	-3.2736307	-2.7743089	2.0551060
H	-2.3514220	-2.2774192	3.5223086
H	-2.5736942	0.0507567	2.9633693
P	1.1023655	-1.5578532	0.4259548
P	-0.8457638	1.2304028	0.1675962
C	2.2673096	-0.2503335	1.0026068
C	2.3359561	0.9458547	0.2590675
C	2.9896123	-0.3840947	2.1976408
C	3.1490498	1.9985399	0.7465921
C	3.7741240	0.6691042	2.6613472
H	2.9551034	-1.3170611	2.7577187
C	3.8538069	1.8634381	1.9492625
H	4.3378213	0.5577157	3.5890256
H	4.4679763	2.6785906	2.3275095
C	0.3012289	1.3848850	-1.2634527
C	-0.1944011	1.6541175	-2.5487252
C	1.6792892	1.1402949	-1.0710593
C	0.6609150	1.6524915	-3.6466110
H	-1.2450525	1.8905663	-2.6956173
C	2.5300081	1.1550100	-2.2060890
C	2.0188329	1.3912696	-3.4876949
H	0.2653702	1.8615825	-4.6417407
H	2.6742320	1.3849640	-4.3567092
C	-4.1531342	-0.2535067	1.5945292
H	-4.9435263	-0.4508613	2.3408185
H	-4.1776569	0.8240018	1.3703998
C	-4.0999969	-2.6124643	-2.7559187
H	-3.4980093	-1.9169189	-3.3551631
H	-3.4756824	-3.4752265	-2.4907167
H	-4.9657669	-2.9475555	-3.3367384
C	1.7951293	-2.0303996	-1.2050517
C	3.1872059	-2.1180115	-1.3749274
C	0.9476990	-2.3455545	-2.2754892
C	3.7192794	-2.5211781	-2.5992949
H	3.8547639	-1.8612309	-0.5507031
C	1.4864442	-2.7364385	-3.5032001
H	-0.1310424	-2.2713760	-2.1479928
C	2.8701983	-2.8266720	-3.6673908
H	4.8015931	-2.5946334	-2.7202411
H	0.8207584	-2.9724199	-4.3351779
H	3.2888505	-3.1378535	-4.6260745
C	1.4578013	-3.0252006	1.4818194
C	1.0814405	-2.9823779	2.8379215
C	2.0025213	-4.2127636	0.9735649
C	1.2659442	-4.0873798	3.6670526
H	0.6462754	-2.0693023	3.2535797
C	2.1725093	-5.3252794	1.8027120
H	2.2917279	-4.2763141	-0.0754479
C	1.8107291	-5.2661948	3.1487420
H	0.9812928	-4.0300733	4.7190223
H	2.5936215	-6.2431348	1.3892208
H	1.9486109	-6.1354568	3.7933944
C	-0.1456091	2.3830752	1.4111544
C	0.2502342	3.6746666	1.0273165
C	-0.0292406	1.9984936	2.7538803
C	0.7421028	4.5663848	1.9797100
H	0.1798981	3.9785535	-0.0184662
C	0.4796413	2.8867887	3.7019703
H	-0.3254203	0.9914657	3.0559773
C	0.8611885	4.1737206	3.3163545
H	1.0383437	5.5717210	1.6754500
H	0.5800781	2.5729093	4.7418880
H	1.2520118	4.8722405	4.0579825
C	-2.4286519	2.0484469	-0.3132189
C	-2.9421333	3.1150100	0.4438330
C	-3.2161932	1.5314080	-1.3592348
C	-4.1986561	3.6544782	0.1554350
H	-2.3648267	3.5286472	1.2701292
C	-4.4658991	2.0782470	-1.6498203
H	-2.8553286	0.6830615	-1.9393927
C	-4.9641182	3.1414058	-0.8922997
H	-4.5758829	4.4838185	0.7559322
H	-5.0559544	1.6655371	-2.4701319
H	-5.9430273	3.5669095	-1.1181767
O	3.8439791	0.9202670	-1.9530799
O	3.1752314	3.1215724	-0.0203476
C	4.0098343	4.2016197	0.3948860
H	3.8920567	4.9771956	-0.3698393
H	3.6929381	4.6004381	1.3726380
H	5.0668610	3.8943341	0.4465465
C	4.7549428	0.9238351	-3.0514324
H	5.7401890	0.7208339	-2.6176193
H	4.5060661	0.1340389	-3.7789601
H	4.7713601	1.9034483	-3.5560989

VR.xyz
98
Energy = -2817.828048253

Rh	-1.3342153	-0.1985650	0.7520498
H	-2.6184471	-1.7688119	-1.2638597
H	-2.5002141	-0.1969011	3.5168143
B	-2.8402072	-0.9815146	-0.3733348
H	-2.6624891	-1.4900340	0.8132754
C	-6.3098120	0.2629873	-1.2014420
C	-5.9143265	1.2176218	-0.3066621
H	-7.2432764	0.1357609	-1.7374049
H	-6.4284289	2.0971422	0.0627192
C	-4.2165224	-0.2344693	-0.5314898
N	-4.6389775	0.8960917	0.0925739
N	-5.2576907	-0.6141618	-1.3347379
C	-2.7320549	1.0831163	1.7482575
C	-3.2965222	0.2776867	2.9227681
H	-3.9681987	-0.5270877	2.5874009
H	-3.8690216	0.9216996	3.6174365
H	-2.1299494	1.9156354	2.1515903
P	0.2939586	-1.8277417	0.3184919
P	-0.1011295	1.5005526	-0.0025684
C	1.7857165	-1.1972710	1.2006191
C	2.5297966	-0.1542107	0.6090136
C	2.0856085	-1.6292965	2.5017902
C	3.5780333	0.4386879	1.3536470
C	3.1173765	-1.0255930	3.2169620
H	1.5233080	-2.4472756	2.9501202
C	3.8622474	0.0098528	2.6566128
H	3.3497853	-1.3691133	4.2263419
H	4.6621953	0.4729964	3.2315182
C	1.2274368	1.0996091	-1.2095927
C	1.1369381	1.5427371	-2.5389834
C	2.3206316	0.3123136	-0.7944186
C	2.1236457	1.1989443	-3.4585190
H	0.3066478	2.1702635	-2.8557793
C	3.3106513	-0.0252015	-1.7507855
C	3.2071021	0.4121280	-3.0769029
H	2.0494227	1.5494923	-4.4891225
H	3.9650959	0.1435490	-3.8104685
C	-3.8232695	1.7758804	0.9613982
H	-4.5527516	2.2618234	1.6354468
H	-3.4068086	2.5560456	0.3113574
C	-5.3130750	-1.8301767	-2.1419140
H	-4.2960570	-2.1306915	-2.4091418
H	-5.7896505	-2.6417721	-1.5759346
H	-5.8933127	-1.6281075	-3.0496805
C	-0.1710232	-3.3862207	1.1781603
C	0.0299838	-4.6619013	0.6316901
C	-0.8278231	-3.2793375	2.4182457
C	-0.4004400	-5.8011114	1.3172030
H	0.5147885	-4.7736553	-0.3379306
C	-1.2438748	-4.4173371	3.1072862
H	-1.0216702	-2.2917007	2.8449154
C	-1.0307693	-5.6842801	2.5566716
H	-0.2398364	-6.7859845	0.8754379
H	-1.7435190	-4.3140000	4.0719315
H	-1.3625059	-6.5764576	3.0900129
C	0.9279067	-2.3806034	-1.3079716
C	2.1142899	-3.1258274	-1.4097554
C	0.2081127	-2.0678029	-2.4690818
C	2.5608942	-3.5633059	-2.6566665
H	2.6965557	-3.3484838	-0.5137443
C	0.6641747	-2.4973984	-3.7161694
H	-0.7031538	-1.4739227	-2.3868192
C	1.8375527	-3.2492474	-3.8113081
H	3.4792915	-4.1490179	-2.7275597
H	0.1048452	-2.2405402	-4.6172945
H	2.1911007	-3.5892899	-4.7861816
C	0.7944214	2.4543013	1.2825492
C	1.7086686	3.4571729	0.9194713
C	0.5977029	2.1619077	2.6401578
C	2.3880406	4.1747330	1.9036657
H	1.8994638	3.6659836	-0.1348850
C	1.2915855	2.8700811	3.6219878
H	-0.0832465	1.3601681	2.9309520
C	2.1805809	3.8830175	3.2552373
H	3.0908497	4.9575451	1.6133696
H	1.1406153	2.6264113	4.6745767
H	2.7175178	4.4426391	4.0230217
C	-1.1690480	2.7134137	-0.8756414
C	-1.2672177	4.0566264	-0.4886820
C	-2.0006777	2.2367646	-1.9061180
C	-2.1833303	4.9061217	-1.1180789
H	-0.6406225	4.4425405	0.3157488
C	-2.9004664	3.0895379	-2.5420391
H	-1.9518702	1.1833462	-2.1907328
C	-2.9988583	4.4278542	-2.1442290
H	-2.2564197	5.9474923	-0.8005977
H	-3.5342892	2.7081766	-3.3446537
H	-3.7102929	5.0942049	-2.6344092
O	4.2528772	1.4357543	0.7216631
O	4.3254301	-0.8019828	-1.2904477
C	5.3634832	-1.1653674	-2.2002285
H	6.0637594	-1.7759430	-1.6199419
H	4.9681821	-1.7591532	-3.0406393
H	5.8860503	-0.2759925	-2.5881781
C	5.3268512	2.0689049	1.4156796
H	5.7236233	2.8197101	0.7234805
H	4.9714023	2.5684028	2.3318560
H	6.1211634	1.3484317	1.6695510

VIR.xyz
98
Energy = -2817.853890877
Rh -1.2749607 -0.0330045   0.3523878
H   -2.6223247   1.0612463   0.8089547
H   -3.7686594 -2.0689801   2.7383297
B   -3.4274166   0.0195069   0.7917429
H   -2.7617345 -1.0752382   0.5623751
C   -6.1306700   0.6969585 -1.8217308
C   -6.7032144   0.9310350 -0.5972727
H   -6.5478886   0.7695278 -2.8197828
H   -7.7037406   1.2562837 -0.3376969
C   -4.5815898   0.2806393 -0.2654144
N   -5.7290758   0.6592241   0.3351525
N   -4.8218615   0.3006901 -1.5950654
C   -4.3501830 -0.0468157   2.1512889
C   -4.6833767 -1.5011298   2.5212117
H   -5.1914373 -2.0200044   1.6921426
H   -5.3390527 -1.5583947   3.4041520
H   -3.8550417   0.4373753   3.0052436
P   0.2754962 -1.6154205   0.1076421
P   0.2373003   1.5652994   0.0669683
C   1.8630370 -1.2834506   0.9760306
C   2.7406963 -0.3147052   0.4484653
C   2.1345307 -1.8885967   2.2124984
C   3.8800267   0.0493502   1.2077068
C   3.2676000 -1.5228793   2.9338489
H   1.4673790 -2.6521237   2.6084674
C   4.1372975 -0.5497213   2.4469794
H   3.4773360 -2.0003828   3.8922911
H   5.0118672 -0.2663576   3.0297716
C   1.5582947   1.2703458 -1.1757747
C   1.4954755   1.8817575 -2.4376224
C   2.5624794   0.3235876 -0.8904125
C   2.4204448   1.5446804 -3.4219556
H   0.7334830   2.6305154 -2.6473924
C   3.4828472 -0.0130136 -1.9136694
C   3.4073318   0.5932509 -3.1739685
H   2.3732358   2.0279240 -4.3991787
H   4.1153776   0.3322385 -3.9584800
C   -5.6377955   0.7421524   1.8059145
H   -6.5517334   0.3214670   2.2505545
H   -5.5677026   1.8033431   2.0882098
C   -3.8474394 -0.0774426 -2.6109045
H   -3.7434969   0.7275474 -3.3496780
H   -2.8861600 -0.2415562 -2.1027770
H   -4.1599266 -1.0016532 -3.1143408
O   4.6653458   1.0136765   0.6578157
O   4.4015119 -0.9590383 -1.5851124
C   5.8288506   1.4245903   1.3745392
H   6.3008733   2.1948516   0.7548386
H   5.5634894   1.8539970   2.3546612

H   6.5307969   0.5867082   1.5156148
C   5.3594287 -1.3405762 -2.5715783
H   5.9884130 -2.0999243 -2.0942017
H   4.8686432 -1.7749879 -3.4580572
H   5.9845447 -0.4856640 -2.8764727
C   -0.6688937   3.0529065 -0.5274421
C   -0.5479058   4.3123071   0.0750619
C   -1.5749796   2.8913191 -1.5908421
C   -1.3136934   5.3885456 -0.3830607
H   0.1374577   4.4569310   0.9104812
C   -2.3275078   3.9683907 -2.0542628
H   -1.6855504   1.9052852 -2.0471689
C   -2.2003565   5.2222944 -1.4476106
H   -1.2134076   6.3626949   0.0982855
H   -3.0180006   3.8321401 -2.8891039
H   -2.7933272   6.0661785 -1.8036858
C   1.1375376   2.1265958   1.5577182
C   2.2369747   2.9939439   1.4536949
C   0.7085964   1.6977168   2.8215124
C   2.8899475   3.4318536   2.6059601
H   2.5927123   3.3107192   0.4716288
C   1.3726652   2.1287559   3.9705739
H   -0.1379400   1.0090382   2.8863672
C   2.4613435   2.9979333   3.8641251
H   3.7406810   4.1103535   2.5205719
H   1.0422479   1.7825928   4.9511549
H   2.9784676   3.3374154   4.7631985
C   -0.3962268 -3.1430966   0.8797768
C   -0.4021404 -4.3895452   0.2383186
C   -0.9822226 -3.0286076   2.1540938
C   -0.9713143 -5.5012703   0.8657123
H   0.0302474 -4.4977320 -0.7564330
C   -1.5348223 -4.1427975   2.7830472
H   -1.0112973 -2.0524233   2.6450093
C   -1.5322078 -5.3834756   2.1381196
H   -0.9735311 -6.4648275   0.3535269
H   -1.9753674 -4.0419198   3.7765206
H   -1.9718669 -6.2548740   2.6258570
C   0.7969312 -2.1262403 -1.5727608
C   1.8830308 -2.9977554 -1.7549974
C   0.0993274 -1.6513679 -2.6907347
C   2.2496866 -3.3972637 -3.0402087
H   2.4519546 -3.3491407 -0.8922629
C   0.4768370 -2.0411691 -3.9760253
H   -0.7231353 -0.9495308 -2.5350875
C   1.5494449 -2.9188828 -4.1517756
H   3.0904886 -4.0801047 -3.1746197
H   -0.0612070 -1.6546813 -4.8432209
H   1.8433706 -3.2279138 -5.1562733

IIIB.xyz
98
Energy = -2817.806229631
Rh -1.3974641   0.8174852 -0.0302421
H   -3.2134769 -1.0716494 -1.4571969
B   -3.0849281   0.0070624 -0.9350211
H   -2.1133635   0.7286448 -1.5990834
C   -4.4130120   0.6868371 -0.5208843
C   -5.9007856   2.1781586   0.2775156
C   -6.5046681   0.9498530   0.2749011
H   -6.2773678   3.1486057   0.5788638
H   -7.4985240   0.6528204   0.5886719
N   -4.6227320   2.0001760 -0.2004289
N   -5.5898232   0.0522298 -0.2257447
C   -3.6039634   3.0495358 -0.3101440
H   -3.4244798   3.2657326 -1.3738625
H   -4.0539788   3.9544711   0.1319260
C   -2.2950664   2.7006962   0.3656343
H   -1.5837370   3.5181852   0.2146149
C   -2.3142062   2.0990820   1.7188000
H   -3.3111485   1.8403722   2.1010095
H   -1.7324333   2.6502413   2.4695545
C   -5.8119850 -1.3855877 -0.3581902
H   -5.4347206 -1.7256834 -1.3287698
H   -5.2855050 -1.9295637   0.4378634
H   -6.8876375 -1.5802082 -0.2905658
P   0.8140477   1.7349480 -0.1206066
P   -0.6059575 -1.3624571   0.0986280
C   1.8957532   0.6972054 -1.1963311
C   2.3431247 -0.5519350 -0.7172212
C   2.1990920   1.0988145 -2.5064923
C   3.1028409 -1.3768648 -1.5839995
C   2.9381500   0.2656543 -3.3417842
H   1.8719437   2.0705174 -2.8721138
C   3.3896353 -0.9733498 -2.8931992
H   3.1719821   0.5874783 -4.3580142
H   3.9626199 -1.6150469 -3.5600202
C   0.8925598 -1.5263870   1.1598020
C   2.1257267 -1.0387811   0.6795031
C   0.7913560 -2.0309967   2.4657490
C   3.2493461 -1.0772876   1.5428748
C   1.9080722 -2.0484393   3.2974439
H   -0.1544116 -2.4286184   2.8301437
C   3.1366429 -1.5697840   2.8486531
H   1.8234598 -2.4469288   4.3098904
H   3.9991898 -1.5866551   3.5123667
C   -0.1437108 -2.2841576 -1.4181496
C   0.4884271 -3.5354042 -1.3203971
C   -0.4189902 -1.7510246 -2.6839119
C   0.8168366 -4.2474764 -2.4737577
H   0.7397867 -3.9443991 -0.3400405
C   -0.0770872 -2.4599194 -3.8362928

H   -0.8807960 -0.7667885 -2.7626364
C   0.5339377 -3.7116412 -3.7336561
H   1.3039496 -5.2204912 -2.3877617
H   -0.2825127 -2.0293720 -4.8176438
H   0.7934669 -4.2692060 -4.6352802
C   -1.8823831 -2.4373879   0.8999298
C   -2.5155196 -1.9665898   2.0648087
C   -2.3212544 -3.6483366   0.3466588
C   -3.5322490 -2.6984721   2.6769550
H   -2.2094773 -1.0118590   2.4971373
C   -3.3563525 -4.3725407   0.9473377
H   -1.8661505 -4.0284669 -0.5676883
C   -3.9604809 -3.9066283   2.1157458
H   -3.9945622 -2.3233946   3.5919485
H   -3.6852839 -5.3109915   0.4975068
H   -4.7597127 -4.4796392   2.5887460
C   0.7771391   3.3870972 -0.9398452
C   1.4075162   4.5272211 -0.4212297
C   -0.0152134   3.5246317 -2.0958706
C   1.2634280   5.7675753 -1.0514527
H   2.0103807   4.4565663   0.4841433
C   -0.1414568   4.7572746 -2.7339748
H   -0.5447524   2.6529596 -2.4879877
C   0.4978698   5.8862433 -2.2112434
H   1.7581462   6.6441777 -0.6297058
H   -0.7458180   4.8393083 -3.6393712
H   0.3929572   6.8540706 -2.7040044
C   1.8747993   2.0037650   1.3568400
C   1.3302000   1.8551474   2.6389577
C   3.2280334   2.3590709   1.2267309
C   2.1128348   2.0723128   3.7740837
H   0.2945361   1.5304732   2.7461590
C   4.0068327   2.5884897   2.3608792
H   3.6750372   2.4424851   0.2344133
C   3.4507862   2.4478868   3.6362360
H   1.6801167   1.9391441   4.7669067
H   5.0555203   2.8699545   2.2486361
H   4.0627821   2.6266678   4.5220076
O   3.5034914 -2.5653294 -1.0566504
O   4.4066088 -0.5973971   1.0157690
C   4.3051874 -3.4238808 -1.8653527
H   4.5311585 -4.2940328 -1.2390660
H   3.7584443 -3.7525127 -2.7646634
H   5.2454918 -2.9321758 -2.1634184
C   5.5817093 -0.6341393   1.8232735
H   5.8368675 -1.6661282   2.1141854
H   6.3822735 -0.2228992   1.1984841
H   5.4663282 -0.0120085   2.7260918
H   -1.7392842   1.0435847   1.7559872

IS.xyz
98
Energy = -2817.830160454
Rh   1.3990501   0.3592530   -0.6150974
P   0.1191050   -1.5258772   -0.5323370
P   -0.3932215   1.5759877   -0.0446164
C   0.2850213   3.1225990   0.6968014
C   -0.0361053   4.3958191   0.2033347
C   1.2438142   3.0176476   1.7228858
C   0.5751646   5.5365275   0.7324855
H   -0.7647865   4.5041600   -0.6003134
C   1.8368229   4.1591038   2.2619349
H   1.5400188   2.0326069   2.0883532
C   1.5054461   5.4239578   1.7660735
H   0.3154773   6.5182385   0.3332098
H   2.5658405   4.0588562   3.0680965
H   1.9734532   6.3169113   2.1831559
C   -1.4253013   0.8157163   1.2815414
C   -2.3019389   -0.2348914   0.9412319
C   -1.2929072   1.2184173   2.6195202
C   -3.0122216   -0.8898235   1.9778505
C   -2.0122581   0.5684352   3.6191537
H   -0.6476121   2.0523497   2.8851905
C   -2.8626357   -0.4902226   3.3117102
H   -1.9089180   0.8916975   4.6561736
H   -3.4072162   -0.9954462   4.1072618
C   -1.6562990   2.1464926   -1.2454262
C   -2.7662357   2.8773929   -0.7881740
C   -1.5442913   1.8457747   -2.6082946
C   -3.7289430   3.3257032   -1.6917727
H   -2.8835484   3.0847990   0.2771709
C   -2.5164988   2.2836623   -3.5079736
H   -0.7105558   1.2340577   -2.9511298
C   -3.6048287   3.0315700   -3.0530829
H   -4.5841466   3.8988593   -1.3296736
H   -2.4282461   2.0311178   -4.5656671
H   -4.3616146   3.3798621   -3.7580202
C   -0.1711620   -2.4848723   1.0046649
C   -1.0638755   -3.5700098   0.9956856
C   0.4890143   -2.1437502   2.1914221
C   -1.2774863   -4.3100496   2.1582129
H   -1.6028623   -3.8266678   0.0818758
C   0.2622615   -2.8788335   3.3559857
H   1.1722185   -1.2950092   2.2000922
C   -0.6170873   -3.9639478   3.3411082
H   -1.9682090   -5.1549651   2.1418889
H   0.7719474   -2.6000291   4.2797510
H   -0.7898802   -4.5406218   4.2515003
C   0.9976491   -2.6841005   -1.6554207
C   1.3786887   -2.2223994   -2.9293619
C   1.3777376   -3.9730363   -1.2577044
C   2.1020056   -3.0424341   -3.7933624

H   1.1101868   -1.2089866   -3.2360173
C   2.1128794   -4.7881071   -2.1228885
H   1.1094273   -4.3430014   -0.2682919
C   2.4724478   -4.3292962   -3.3907268
H   2.3825139   -2.6746535   -4.7817871
H   2.4039447   -5.7889927   -1.7998973
H   3.0435662   -4.9703225   -4.0641090
C   -1.5763251   -1.3599501   -1.2240707
C   -1.8827310   -1.8173390   -2.5145270
C   -2.5453387   -0.6801284   -0.4608537
C   -3.1487192   -1.5895831   -3.0489896
H   -1.1420036   -2.3647983   -3.0947549
C   -3.8198234   -0.4457593   -1.0314681
C   -4.1172655   -0.8999533   -2.3226440
H   -3.3871322   -1.9553661   -4.0490869
H   -5.0967774   -0.7208712   -2.7622980
O   -4.6899826   0.2496828   -0.2537406
O   -3.8086136   -1.9157177   1.5821034
C   -5.9895567   0.5240184   -0.7755901
H   -6.5104209   1.0840639   0.0086720
H   -5.9305277   1.1397491   -1.6881750
H   -6.5409765   -0.4056669   -0.9900332
C   -4.5375156   -2.6288169   2.5807521
H   -5.0970905   -3.4010715   2.0418330
H   -3.8572916   -3.1067189   3.3045784
H   -5.2423887   -1.9687867   3.1117622
C   6.6843369   1.0228274   1.0409463
C   6.0663040   2.0452558   0.3850643
C   4.5964314   0.3373058   0.5199182
N   5.7743285   -0.0152516   1.1077719
H   7.6855375   0.9438755   1.4472260
H   6.4271019   3.0276323   0.1045582
N   4.7917698   1.6112940   0.0745835
C   3.8050851   2.4311587   -0.6539240
H   4.3965339   3.1628288   -1.2293100
H   3.1914827   2.9912300   0.0668207
C   2.9732736   1.5943516   -1.5768687
H   3.5605903   0.8774898   -2.1593869
C   1.7290497   1.9634750   -2.1044487
H   1.2699822   2.9145828   -1.8272818
H   1.4464738   1.5888317   -3.0887227
C   6.0406181   -1.3083771   1.7314601
B   3.2715826   -0.5265726   0.5016115
H   3.4017514   -1.5996507   1.0407088
H   2.3687822   0.1275384   1.0945099
H   2.8993972   -0.8036791   -0.6966276
H   5.7771814   -2.1174334   1.0415602
H   7.1076195   -1.3635598   1.9726592
H   5.4504574   -1.4193686   2.6495250

IIS.xyz
98
Energy = -2817.825872054

Rh	-1.4895445	0.3631707	-0.2013203
H	-2.8000566	-0.7094326	-0.9746922
H	-2.7848327	-0.5188914	1.0929283
B	-3.4704996	-0.8966294	0.1137283
H	-3.6298949	-2.0907660	0.1489178
C	-6.9769543	0.5370901	-0.0694181
C	-6.2967887	1.5817448	0.4819939
H	-8.0250822	0.4294360	-0.3218531
H	-6.6373529	2.5587167	0.8033469
C	-4.8165354	-0.0847061	0.1191629
N	-4.9776091	1.1819467	0.5942348
N	-6.0568543	-0.4740364	-0.2840161
C	-2.7308312	2.1798723	0.1794192
C	-2.7734770	1.8675586	-1.1775187
H	-3.6466633	1.3747464	-1.6060528
H	-2.1572595	2.4152774	-1.8841078
H	-2.0418680	2.9562158	0.5226928
P	-0.1536500	-1.5677550	0.0147535
P	0.3818707	1.6686777	-0.2173642
C	1.2649695	-1.4063281	1.1835952
C	2.3657175	-0.6048121	0.8261807
C	1.2076413	-1.9851766	2.4618974
C	3.3764591	-0.3663841	1.7924841
C	2.2156812	-1.7448256	3.3899969
H	0.3897959	-2.6476095	2.7318253
C	3.2941879	-0.9236170	3.0726611
H	2.1608064	-2.2052598	4.3776808
H	4.0685609	-0.7340372	3.8137111
C	1.8872589	1.0335282	-1.0888214
C	2.2821167	1.5601743	-2.3299017
C	2.5949954	-0.0533743	-0.5401244
C	3.3377941	0.9944274	-3.0370050
H	1.7901872	2.4361188	-2.7415849
C	3.6562153	-0.6262432	-1.2876694
C	4.0187622	-0.1114983	-2.5358228
H	3.6346662	1.4214766	-3.9962062
H	4.8318567	-0.5545575	-3.1078363
C	-3.8884961	1.9887749	1.1340041
H	-3.5457168	1.5413828	2.0803101
H	-4.3158064	2.9744057	1.3766550
C	-1.0856358	-3.0329692	0.6247048
C	-1.2236779	-4.1900994	-0.1548297
C	-1.7391880	-2.9781976	1.8689450
C	-1.9697806	-5.2754581	0.3122294
H	-0.7535793	-4.2518263	-1.1355568
C	-2.4646143	-4.0694437	2.3422197
H	-1.7051526	-2.0648880	2.4639144
C	-2.5813323	-5.2245479	1.5648493
H	-2.0658472	-6.1667169	-0.3100174
H	-2.9541609	-4.0101505	3.3156285
H	-3.1549756	-6.0772541	1.9315454
C	0.5877054	-2.1440820	-1.5537893
C	0.1622159	-1.5949836	-2.7704448
C	1.5514038	-3.1658549	-1.5496425
C	0.6986663	-2.0580166	-3.9730002
H	-0.5804740	-0.7931529	-2.7597188
C	2.0759339	-3.6320739	-2.7541880
H	1.8983004	-3.5860494	-0.6042141
C	1.6533706	-3.0772996	-3.9663628
H	0.3710894	-1.6205362	-4.9173348
H	2.8192163	-4.4312585	-2.7465303
H	2.0697090	-3.4412896	-4.9071568
C	0.1170284	3.3411749	-0.9642554
C	0.1703334	4.5132462	-0.1932752
C	-0.2305804	3.4561787	-2.3248460
C	-0.0872349	5.7602698	-0.7696569
H	0.4207804	4.4602922	0.8660821
C	-0.4722987	4.7025259	-2.9023427
H	-0.3148321	2.5591133	-2.9419387
C	-0.3995062	5.8611279	-2.1253245
H	-0.0361989	6.6573211	-0.1503762
H	-0.7255605	4.7659065	-3.9618432
H	-0.5916479	6.8364277	-2.5748472
C	1.0198008	2.0814716	1.4578408
C	0.2717418	1.7323219	2.5896273
C	2.2336713	2.7695609	1.6177849
C	0.7283512	2.0621532	3.8669260
H	-0.6608934	1.1775926	2.4534742
C	2.6810148	3.1098956	2.8937820
H	2.8328577	3.0290563	0.7432349
C	1.9315033	2.7546451	4.0200064
H	0.1467616	1.7738063	4.7440596
H	3.6211979	3.6519924	3.0103893
H	2.2875819	3.0173273	5.0175909
O	4.2634978	-1.6974009	-0.7098658
O	4.3952480	0.4365429	1.3848827
C	5.3559559	-2.3045976	-1.3983474
H	5.6899129	-3.1265103	-0.7556473
H	5.0395550	-2.7076148	-2.3745686
H	6.1842010	-1.5923307	-1.5442730
C	5.4548191	0.6991596	2.3036974
H	6.1553597	1.3494231	1.7684304
H	5.0849961	1.2196450	3.2025022
H	5.9688187	-0.2296600	2.5998982
C	-6.3666324	-1.7562639	-0.9054204
H	-6.4746031	-1.6362795	-1.9920183
H	-5.5470881	-2.4510658	-0.6970847
H	-7.3008741	-2.1491073	-0.4863933

IIIS.xyz
98
Energy = -2817.812577848
Rh -1.2998491   0.5539473 -0.6547013
H   -2.3755416 -0.5706951 -1.0208553
H   -2.2100393   2.2630944   1.3591146
B   -2.6299749   1.1679098   1.0501613
H   -2.5668487   0.3348180   1.9170103
C   -6.0738330   0.8925196 -0.5139156
C   -5.5462738   1.9637574 -1.1784457
H   -7.0403124   0.4109822 -0.6040139
H   -5.9594946   2.5827386 -1.9661770
C   -4.0097318   1.2552810   0.3152164
N   -4.2926020   2.1779366 -0.6473422
N   -5.1205047   0.4727236   0.3959594
C   -2.1148320   2.3648166 -1.7813599
C   -2.2978821   1.1687210 -2.4806200
H   -3.2923701   0.7409415 -2.6113620
H   -1.5639045   0.8702493 -3.2357934
H   -1.2690147   3.0112413 -2.0211664
P   -0.5506497 -1.4757712   0.1585175
P   0.6092847   1.8064215 -0.0442337
C   1.0800212 -1.5547046   1.0230735
C   2.1973775 -0.9380688   0.4235008
C   1.2224398 -2.2107275   2.2558016
C   3.4324339 -0.9442025   1.1131769
C   2.4531463 -2.2218536   2.9065183
H   0.3788805 -2.7283865   2.7063327
C   3.5573455 -1.5769038   2.3552965
H   2.5534047 -2.7368264   3.8631926
H   4.5065691 -1.5769640   2.8880187
C   1.5948160   0.8778756 -1.2810853
C   1.5455403   1.3041667 -2.6248926
C   2.1721870 -0.3650275 -0.9548304
C   2.1079723   0.5213029 -3.6267717
H   1.0667798   2.2488585 -2.8826177
C   2.7632920 -1.1319850 -1.9912625
C   2.7260178 -0.6906406 -3.3197819
H   2.0713960   0.8585103 -4.6639048
H   3.1641166 -1.2899380 -4.1158060
C   -3.2696090   3.0988762 -1.1327369
H   -2.9183357   3.7061076 -0.2875888
H   -3.7490035   3.7792453 -1.8541842
C   -1.7221162 -2.3912461   1.2361075
C   -2.5030391 -3.4282969   0.7031206
C   -1.9258796 -2.0087172   2.5737535
C   -3.4548077 -4.0776311   1.4926830
H   -2.3633263 -3.7388207 -0.3330434
C   -2.8697345 -2.6675165   3.3634810
H   -1.3400499 -1.1989442   3.0079595
C   -3.6381959 -3.7031391   2.8254567
H   -4.0456955 -4.8890202   1.0643129
H   -3.0045032 -2.3669078   4.4038325
H   -4.3726966 -4.2197952   3.4452538
C   -0.2557400 -2.6410357 -1.2391048
C   0.4927626 -3.8076413 -1.0072925
C   -0.7747882 -2.4068306 -2.5193189
C   0.7011024 -4.7254468 -2.0357238
H   0.9177580 -3.9965248 -0.0203918
C   -0.5521181 -3.3207808 -3.5518025
H   -1.3584697 -1.5053540 -2.7041416
C   0.1828948 -4.4828523 -3.3116841
H   1.2757980 -5.6324493 -1.8405708
H   -0.9568949 -3.1229226 -4.5456339
H   0.3515508 -5.2007246 -4.1162225
C   0.8114627   3.5916010 -0.4214827
C   -0.1255649   4.4565467   0.1693003
C   1.8775865   4.1373286 -1.1521849
C   -0.0099070   5.8377092   0.0167268
H   -0.9345449   4.0392356   0.7735959
C   1.9858616   5.5214341 -1.3088952
H   2.6302178   3.4858360 -1.5979698
C   1.0429457   6.3733134 -0.7304419
H   -0.7402519   6.4982958   0.4870443
H   2.8177402   5.9345785 -1.8817717
H   1.1330439   7.4535544 -0.8536650
C   1.4289771   1.7610016   1.5922287
C   2.7326745   2.2557781   1.7565090
C   0.7006634   1.3363905   2.7104121
C   3.3065755   2.2966575   3.0254499
H   3.3006407   2.6043952   0.8925409
C   1.2791037   1.3832792   3.9805426
H   -0.3226889   0.9809220   2.5798490
C   2.5817399   1.8590854   4.1392315
H   4.3204059   2.6817978   3.1490106
H   0.7075403   1.0508965   4.8486462
H   3.0314967   1.8991272   5.1325942
O   3.3301546 -2.3016302 -1.5995430
O   4.4455960 -0.2858323   0.4900097
C   5.7212951 -0.2546274   1.1314013
H   6.3746939   0.3156520   0.4623737
H   5.6638416   0.2516823   2.1089005
H   6.1284948 -1.2699896   1.2642453
C   3.9196735 -3.1358083 -2.5976009
H   4.3052989 -4.0089652 -2.0602655
H   3.1704222 -3.4633166 -3.3361675
H   4.7508368 -2.6234141 -3.1083217
C   -5.2762854 -0.6718314   1.2852720
H   -5.3469409 -1.5961256   0.6971266
H   -4.3981853 -0.7310200   1.9340723
H   -6.1808394 -0.5512883   1.8947540

IVS.xyz
98
Energy = -2817.816724416

Rh	-1.3156631	-0.3257486	-0.7449240
H	-2.3714678	-1.8995634	-1.0327944
H	-2.4822376	2.0017362	0.4176387
B	-2.6312725	0.8141939	0.6443916
H	-2.3087605	0.4701386	1.7584265
C	-6.2736222	-0.2279425	0.4027142
C	-6.0183884	0.1636460	-0.8812158
H	-7.1832160	-0.5935352	0.8640755
H	-6.6575589	0.1875708	-1.7558250
C	-4.1141031	0.4134242	0.3009432
N	-4.6977293	0.5582156	-0.9166407
N	-5.0939299	-0.0793273	1.1096613
C	-2.7309884	-0.0462406	-2.2462662
C	-2.9672647	-1.5066591	-1.9615265
H	-3.9943255	-1.7617543	-1.6625565
H	-2.6345311	-2.1831227	-2.7585044
H	-2.2366674	0.1324276	-3.2077491
P	0.1124814	-1.5479993	0.6708596
P	-0.0277309	1.4792936	-0.8648370
C	1.5185422	-0.7242801	1.5127471
C	2.3923278	0.0371599	0.7123408
C	1.7002969	-0.7863189	2.9021274
C	3.4301130	0.7621459	1.3500225
C	2.7306326	-0.0695407	3.5041960
H	1.0473408	-1.4045204	3.5151069
C	3.5876409	0.7188027	2.7402842
H	2.8690736	-0.1230733	4.5852461
H	4.3793499	1.2854011	3.2269611
C	1.5079835	0.7758206	-1.6110143
C	1.7200727	0.8204727	-2.9994415
C	2.3916220	0.0407991	-0.7856346
C	2.7709907	0.1151410	-3.5773101
H	1.0851749	1.4329267	-3.6328338
C	3.4438109	-0.6835580	-1.4044964
C	3.6220474	-0.6583304	-2.7926270
H	2.9294346	0.1665859	-4.6556699
H	4.4289917	-1.2201495	-3.2595410
C	-3.9087659	0.9034372	-2.0969121
H	-3.5490488	1.9401946	-2.0024821
H	-4.5935073	0.8636411	-2.9601500
C	-4.9390914	-0.3570697	2.5333608
H	-3.9750535	-0.8477649	2.7049639
H	-4.9796294	0.5742737	3.1133817
H	-5.7500259	-1.0215587	2.8515197
C	-0.8023254	-2.4725243	1.9649528
C	-1.0880731	-3.8386480	1.8086229
C	-1.3449312	-1.7916432	3.0708130
C	-1.8823941	-4.5097785	2.7411071
H	-0.6820158	-4.3866810	0.9573581

C	-2.1223376	-2.4705604	4.0100023
H	-1.1562989	-0.7259847	3.2018243
C	-2.3965931	-3.8314789	3.8475425
H	-2.0882863	-5.5728427	2.6056583
H	-2.5126162	-1.9327214	4.8763683
H	-3.0031790	-4.3611994	4.5836511
C	0.9698776	-2.8560555	-0.2952504
C	1.9558150	-3.6588493	0.3002651
C	0.6670040	-3.0393330	-1.6514832
C	2.6077938	-4.6396584	-0.4461685
H	2.2186974	-3.5077210	1.3489327
C	1.3275293	-4.0136120	-2.4021857
H	-0.0746797	-2.3963241	-2.1328210
C	2.2954067	-4.8185973	-1.7978834
H	3.3685178	-5.2632779	0.0266025
H	1.0902368	-4.1397805	-3.4596254
H	2.8100475	-5.5845851	-2.3804519
C	-0.7207448	2.8005824	-1.9515929
C	-1.0815063	4.0379996	-1.3910313
C	-1.0546287	2.5613981	-3.2976735
C	-1.7244391	5.0115160	-2.1591402
H	-0.8631317	4.2473761	-0.3446265
C	-1.6775708	3.5422557	-4.0690567
H	-0.8450049	1.5957672	-3.7542477
C	-2.0143075	4.7741442	-3.5027373
H	-1.9948601	5.9631712	-1.6988995
H	-1.9072567	3.3376813	-5.1161445
H	-2.5060948	5.5398804	-4.1044218
C	0.6157521	2.4618220	0.5465980
C	1.6271871	3.3970106	0.2662208
C	0.1314505	2.3399032	1.8533662
C	2.1388204	4.2012335	1.2830739
H	2.0189912	3.4922223	-0.7481339
C	0.6563696	3.1387116	2.8706005
H	-0.6549999	1.6203261	2.0717945
C	1.6563723	4.0715808	2.5887177
H	2.9183420	4.9299765	1.0542163
H	0.2806948	3.0299347	3.8892118
H	2.0594791	4.6993436	3.3851683
O	4.2281591	1.4876334	0.5222046
O	4.2423789	-1.3853256	-0.5583269
C	5.2937366	2.2394943	1.1017209
H	5.7964414	2.7337077	0.2632655
H	4.9105181	3.0011891	1.8004574
H	6.0093237	1.5843980	1.6245832
C	5.3087203	-2.1544369	-1.1135908
H	5.8031740	-2.6300164	-0.2596263
H	4.9267308	-2.9330353	-1.7938223
H	6.0313602	-1.5149798	-1.6459751

VS.xyz
98
Energy = -2817.818912203

Rh	-1.5211090	-0.1254705	-0.8394756
H	-3.6925787	-0.3628069	-2.8496410
H	-2.2032493	-1.1990694	1.6964543
B	-2.6828937	-0.5667329	0.7795394
H	-2.9369428	-1.2696127	-0.2754321
C	-5.5806496	1.1784265	2.4725699
C	-5.3436664	2.0380081	1.4363629
H	-6.3201622	1.2085553	3.2642423
H	-5.8241920	2.9709684	1.1665293
C	-3.8711645	0.3506640	1.2617829
N	-4.2991119	1.5138525	0.7106050
N	-4.6641382	0.1559506	2.3571874
C	-3.0732749	1.1940312	-1.4386337
C	-4.1397192	0.3597374	-2.1496226
H	-4.7618150	-0.2160590	-1.4480278
H	-4.8149182	1.0026218	-2.7454173
H	-2.5570430	1.8166918	-2.1852023
P	0.0444932	-1.8994236	-0.6213380
P	-0.0036042	1.4757267	-0.4441705
C	1.0508114	-1.6779245	0.9001176
C	1.9951898	-0.6298176	0.9391038
C	0.7581694	-2.4078445	2.0616441
C	2.6218917	-0.3310994	2.1741725
C	1.3824657	-2.0892580	3.2649827
H	0.0571539	-3.2394069	2.0236222
C	2.3030675	-1.0464422	3.3350459
H	1.1539137	-2.6655966	4.1631371
H	2.7795073	-0.8071371	4.2839760
C	1.7394675	1.1164439	-0.9425576
C	2.3218608	1.8077983	-2.0182389
C	2.4691917	0.1153202	-0.2680939
C	3.6132408	1.5033306	-2.4360192
H	1.7788018	2.6040630	-2.5208791
C	3.7800185	-0.1825602	-0.7218771
C	4.3455121	0.5039172	-1.8021347
H	4.0562014	2.0516403	-3.2688333
H	5.3497117	0.2657708	-2.1478551
C	-3.6697384	2.1722441	-0.4517474
H	-2.9052357	2.8647431	-0.0691659
H	-4.4703760	2.7802964	-0.9111840
C	-4.6190036	-1.0122307	3.2310231
H	-5.2468551	-1.8177412	2.8270089
H	-3.5853010	-1.3655007	3.3045338
H	-4.9850668	-0.7274660	4.2237407
C	-0.3863353	3.0542268	-1.3197670
C	-0.5921610	4.2693579	-0.6512974
C	-0.5697754	3.0140616	-2.7152624
C	-0.9543279	5.4178491	-1.3620264
H	-0.4693753	4.3276596	0.4304257

C	-0.9160532	4.1630127	-3.4244392
H	-0.4376256	2.0720058	-3.2535236
C	-1.1112889	5.3705858	-2.7473926
H	-1.1079513	6.3552813	-0.8249204
H	-1.0422334	4.1132636	-4.5070800
H	-1.3880783	6.2696343	-3.2999489
C	0.2167130	1.9954729	1.3058930
C	1.2800586	2.8612192	1.6187690
C	-0.6444454	1.5798683	2.3262790
C	1.4537584	3.3162929	2.9253285
H	1.9793861	3.1713816	0.8407900
C	-0.4607903	2.0249242	3.6360849
H	-1.4404973	0.8740320	2.0928278
C	0.5850039	2.8994646	3.9378419
H	2.2794399	3.9921761	3.1542310
H	-1.1319791	1.6800511	4.4245288
H	0.7278472	3.2518769	4.9607654
C	1.2592126	-2.0975000	-1.9778386
C	2.3911294	-2.9154842	-1.8306524
C	1.0171005	-1.4739790	-3.2088122
C	3.2629341	-3.1024752	-2.9025196
H	2.5910836	-3.3985188	-0.8726222
C	1.8942229	-1.6571876	-4.2794057
H	0.1360843	-0.8367905	-3.3267436
C	3.0173381	-2.4729661	-4.1270560
H	4.1367190	-3.7457693	-2.7836211
H	1.7005587	-1.1633164	-5.2327982
H	3.7017911	-2.6203765	-4.9639760
C	-0.7178787	-3.5819044	-0.5418582
C	-0.4050592	-4.5682786	-1.4925991
C	-1.7020855	-3.8762859	0.4202560
C	-1.0376620	-5.8134980	-1.4659586
H	0.3336037	-4.3708914	-2.2679378
C	-2.3206686	-5.1252904	0.4530574
H	-2.0001590	-3.1196641	1.1439530
C	-1.9907491	-6.1016400	-0.4898107
H	-0.7780554	-6.5607640	-2.2176163
H	-3.0720542	-5.3336309	1.2169939
H	-2.4799265	-7.0766002	-0.4676654
O	3.5302934	0.6814027	2.1390327
O	4.4158491	-1.1802705	-0.0522908
C	4.2109293	1.0189548	3.3460661
H	4.8923427	1.8354302	3.0824646
H	3.5062079	1.3666402	4.1193561
H	4.7928952	0.1660704	3.7313904
C	5.7476843	-1.5138801	-0.4423033
H	6.0572723	-2.3228002	0.2283369
H	5.7827410	-1.8685656	-1.4854503
H	6.4281554	-0.6554699	-0.3213126

VIS.xyz
98
Energy = -2817.854979644

Rh	-1.3199331	0.1463231	-0.1545995
H	-2.7797715	0.1478931	-3.3698136
H	-2.7465353	1.2580464	-0.3049812
B	-3.4797659	0.2014750	-0.5197965
H	-2.7494195	-0.8960384	-0.4777698
C	-6.2488496	-0.2064514	2.0763171
C	-6.8334728	-0.4004197	0.8506307
H	-6.6759581	-0.2348887	3.0723825
H	-7.8572387	-0.6399420	0.5884519
C	-4.6618765	0.0608840	0.5263813
N	-5.8346767	-0.2227678	-0.0789918
N	-4.9093424	0.0729380	1.8541415
C	-4.3666637	0.2769398	-1.8963615
C	-3.7373282	-0.3433033	-3.1434563
H	-3.5237603	-1.4121285	-2.9884502
H	-4.3787903	-0.2486988	-4.0335921
H	-4.5393993	1.3518236	-2.0897055
P	0.1485219	-1.5040323	0.0835492
P	0.3000847	1.6727240	-0.0998939
C	1.5981729	-1.2156322	1.1741004
C	2.6043997	-0.3254901	0.7483832
C	1.6405011	-1.7739161	2.4610897
C	3.6380138	0.0089580	1.6574960
C	2.6740082	-1.4394073	3.3317506
H	0.8739134	-2.4783289	2.7793132
C	3.6677825	-0.5433103	2.9442622
H	2.7074124	-1.8807082	4.3291426
H	4.4621569	-0.2830816	3.6414711
C	1.7780915	1.2370850	-1.1039923
C	1.9377071	1.7759477	-2.3898828
C	2.6669820	0.2517631	-0.6281304
C	2.9702495	1.3291973	-3.2096756
H	1.2611834	2.5499902	-2.7479850
C	3.7029915	-0.1935137	-1.4856755
C	3.8486185	0.3404549	-2.7720209
H	3.0932421	1.7544403	-4.2069816
H	4.6433020	-0.0060585	-3.4301941
C	-5.7419283	-0.3436635	-1.5456095
H	-6.6021804	0.1580850	-2.0106567
H	-5.7807396	-1.4128689	-1.8089461
C	-3.9071273	0.3620757	2.8729621
H	-3.8522400	-0.4667441	3.5903488
H	-2.9389134	0.4765364	2.3654441
H	-4.1585327	1.2910772	3.4008483
O	4.5045127	-1.1674929	-0.9776332
O	4.5557218	0.8996667	1.1969438
C	5.5661329	-1.6599704	-1.7940469
H	6.0717122	-2.4232443	-1.1924243
H	5.1791480	-2.1186594	-2.7188923
H	6.2813064	-0.8610152	-2.0487064
C	5.6264687	1.2729742	2.0631792
H	6.2338594	1.9840025	1.4925692
H	5.2497774	1.7623359	2.9765573
H	6.2431445	0.4019564	2.3381620
C	-0.3747851	3.2060898	-0.8613018
C	-0.2155811	4.4786775	-0.2954398
C	-1.1275522	3.0748651	-2.0429436
C	-0.7893616	5.5974035	-0.9059402
H	0.3486935	4.6027130	0.6288542
C	-1.6874025	4.1940766	-2.6560956
H	-1.2795194	2.0818511	-2.4733157
C	-1.5203854	5.4602562	-2.0867212
H	-0.6621485	6.5815446	-0.4519784
H	-2.2604372	4.0773397	-3.5775702
H	-1.9644598	6.3369122	-2.5609171
C	0.9894790	2.2119801	1.5083546
C	2.1379490	3.0178196	1.5696173
C	0.3504452	1.8295592	2.6950548
C	2.6265558	3.4437143	2.8048274
H	2.6597231	3.2954472	0.6520365
C	0.8493172	2.2458765	3.9297266
H	-0.5270919	1.1811177	2.6322084
C	1.9854149	3.0571073	3.9855625
H	3.5156463	4.0755233	2.8457894
H	0.3554321	1.9327343	4.8510558
H	2.3747503	3.3857320	4.9506097
C	-0.7589165	-2.9113801	0.8454385
C	-0.7452194	-4.2077211	0.3135841
C	-1.5535160	-2.6464544	1.9753408
C	-1.5067517	-5.2195238	0.9059051
H	-0.1472282	-4.4312198	-0.5701750
C	-2.3008474	-3.6598384	2.5720165
H	-1.5802753	-1.6311457	2.3778841
C	-2.2815687	-4.9512911	2.0350842
H	-1.4908868	-6.2238249	0.4794617
H	-2.9019171	-3.4449183	3.4578767
H	-2.8711539	-5.7453162	2.4960200
C	0.8675067	-2.1814396	-1.4562422
C	1.9402655	-3.0865957	-1.4177282
C	0.3230435	-1.8022374	-2.6912465
C	2.4523659	-3.6103329	-2.6049371
H	2.3860233	-3.3660031	-0.4614045
C	0.8460747	-2.3200237	-3.8766539
H	-0.5007678	-1.0842501	-2.7069432
C	1.9090700	-3.2257719	-3.8345579
H	3.2829029	-4.3176914	-2.5699378
H	0.4257094	-2.0128505	-4.8355897
H	2.3167297	-3.6323273	-4.7616813

Ts0_IR.xyz
98
Energy = -2817.809595906

Rh	-1.2797532	0.2274992	-0.0121591
P	0.0509398	-1.4431781	0.4662597
P	0.4464746	1.5880406	-0.2952234
C	-0.2242080	3.0922289	-1.1190828
C	-0.0222538	4.3826006	-0.6051849
C	-1.0443693	2.9344608	-2.2522411
H	0.5952172	4.5300503	0.2806587
C	-0.6111847	5.4893497	-1.2218112
H	-1.2459143	1.9333655	-2.6379267
C	-1.4022860	5.3250031	-2.3595842
H	-0.4458745	6.4855602	-0.8082281
H	-2.2375635	3.9043635	-3.7605728
H	-1.8557807	6.1922751	-2.8420688
C	1.6997810	0.8590131	-1.4274666
C	2.5553678	-0.1433267	-0.9256134
C	1.7081432	1.1816751	-2.7925234
C	3.3866068	-0.8396662	-1.8374317
C	2.5466181	0.4941180	-3.6657282
H	1.0696469	1.9768349	-3.1731563
C	3.3749712	-0.5256115	-3.2021161
H	2.5540989	0.7523887	-4.7258787
H	4.0127504	-1.0637344	-3.9009985
C	1.4658548	2.2534004	1.0778503
C	2.6233504	2.9962908	0.7905967
C	1.0983719	2.0424479	2.4119424
C	3.3857699	3.5326924	1.8276806
H	2.9339930	3.1435036	-0.2454496
C	1.8697935	2.5691122	3.4487507
H	0.2194035	1.4362857	2.6307502
C	3.0111766	3.3196139	3.1579578
H	4.2794457	4.1149245	1.5960634
H	1.5829960	2.3867959	4.4855842
H	3.6126153	3.7355538	3.9679707
C	0.4722965	-2.5055053	-0.9684972
C	1.4264740	-3.5275795	-0.8355337
C	-0.1599722	-2.3025394	-2.2025738
C	1.7335800	-4.3409546	-1.9263823
H	1.9404371	-3.6765898	0.1157991
C	0.1602678	-3.1108870	-3.2941265
H	-0.8874665	-1.4932085	-2.2964624
C	1.1049374	-4.1310852	-3.1575089
H	2.4727549	-5.1364516	-1.8162833
H	-0.3256539	-2.9399627	-4.2561263
H	1.3535463	-4.7637986	-4.0113998
C	-0.8792505	-2.5349101	1.6176741
C	-1.3644838	-1.9854164	2.8187987
C	-1.2127147	-3.8571585	1.2938002
C	-2.1488253	-2.7463386	3.6836807
H	-1.1193203	-0.9524640	3.0746205
C	-2.0104145	-4.6143966	2.1568638
H	-0.8565235	-4.2979624	0.3623775
C	-2.4781481	-4.0648349	3.3511273
H	-2.5050551	-2.3105882	4.6189318
H	-2.2639357	-5.6420330	1.8912627
H	-3.0969304	-4.6608794	4.0237079
C	1.6825722	-1.1588584	1.2580822
C	1.9038657	-1.5136210	2.5980770
C	2.6779339	-0.4825049	0.5245259
C	3.1064053	-1.1831101	3.2166105
H	1.1451313	-2.0611998	3.1542128
C	3.8842053	-0.1381432	1.1834042
C	4.0935551	-0.4859574	2.5238689
H	3.2784987	-1.4687564	4.2555865
H	5.0213592	-0.2203723	3.0273692
O	4.7816839	0.5545299	0.4345562
O	4.1596990	-1.8169771	-1.2940341
C	6.0153595	0.9357746	1.0420480
H	6.5727353	1.4724676	0.2666371
H	5.8465505	1.6045058	1.9022341
H	6.5932033	0.0549060	1.3657355
C	5.0085408	-2.5660956	-2.1623509
H	5.5284656	-3.2845364	-1.5191547
H	4.4222157	-3.1104033	-2.9208370
H	5.7481285	-1.9179530	-2.6599153
C	-7.0746132	0.0551960	-0.6159224
C	-6.7095082	0.3022190	0.6748836
C	-4.8219581	-0.0208695	-0.5171492
N	-5.9093372	-0.1423331	-1.3290809
H	-8.0533352	0.0002336	-1.0772005
H	-7.3084915	0.5041472	1.5548601
N	-5.3308624	0.2488751	0.7176032
C	-4.5331526	0.5176175	1.9239865
H	-3.8287001	-0.3142565	2.0714406
H	-5.2443035	0.5120731	2.7644395
C	-3.8007790	1.8249319	1.8349154
H	-4.3716514	2.6791082	1.4586241
C	-2.5156784	1.9584667	2.1802158
H	-1.9474904	1.1105216	2.5669588
H	-2.0037719	2.9194433	2.1302709
C	-5.8590050	-0.4299788	-2.7607753
B	-3.3099906	-0.1598374	-0.9728615
H	-3.2443572	-0.6805188	-2.0630682
H	-2.7834616	0.9959384	-0.9928531
H	-2.7197765	-0.9005046	-0.0857254
H	-5.3532362	-1.3862801	-2.9357483
H	-6.8856014	-0.4815884	-3.1384915
H	-5.3144536	0.3624127	-3.2873927

Ts0_IIR.xyz
98
Energy = -2817.816094756

Rh	-0.9895090	-0.9347112	-0.6905620
P	1.1718695	-0.9547282	-0.2820072
P	-1.0728194	1.2609763	-0.3986089
C	-2.7109868	1.8073736	-1.0362148
C	-3.5711461	2.6406277	-0.3046630
C	-3.1512544	1.2899636	-2.2692662
C	-4.8384252	2.9571640	-0.8016985
H	-3.2590778	3.0419782	0.6594669
C	-4.4102573	1.6197823	-2.7680539
H	-2.5060226	0.6096877	-2.8297557
C	-5.2590182	2.4535976	-2.0334827
H	-5.4976648	3.6033013	-0.2196818
H	-4.7326957	1.2177118	-3.7298702
H	-6.2478816	2.7056330	-2.4197660
C	0.2101205	2.1118062	-1.4037693
C	1.5480994	2.0878702	-0.9577722
C	-0.1086527	2.6267073	-2.6689034
C	2.5587537	2.5591241	-1.8310624
C	0.9017009	3.0985541	-3.5026992
H	-1.1448780	2.6654422	-3.0008729
C	2.2348755	3.0551431	-3.1003427
H	0.6496332	3.5025238	-4.4844488
H	3.0132269	3.4151943	-3.7707270
C	-0.9490928	2.0480079	1.2504366
C	-0.8281260	3.4421294	1.3716844
C	-0.9985610	1.2550303	2.4032488
C	-0.7743443	4.0302472	2.6352000
H	-0.7604263	4.0643861	0.4773436
C	-0.9302423	1.8458308	3.6659770
H	-1.0751850	0.1713650	2.2942316
C	-0.8234605	3.2337030	3.7835610
H	-0.6883343	5.1147132	2.7238315
H	-0.9505264	1.2212720	4.5610048
H	-0.7734472	3.6960861	4.7707304
C	2.2537455	-0.9324825	-1.7581431
C	3.6423618	-0.7658576	-1.6285586
C	1.6878445	-1.0775992	-3.0330447
C	4.4523061	-0.7590846	-2.7644724
H	4.0867283	-0.6216316	-0.6421139
C	2.5012059	-1.0584151	-4.1665507
H	0.6037296	-1.1813467	-3.1229250
C	3.8833210	-0.9019245	-4.0334774
H	5.5312354	-0.6330367	-2.6582187
H	2.0540903	-1.1602176	-5.1565900
H	4.5189877	-0.8883081	-4.9205202
C	1.4808639	-2.5670642	0.5506584
C	0.6551511	-2.9116412	1.6376836
C	2.4562174	-3.4768776	0.1190818
C	0.8240096	-4.1290804	2.2962296
H	-0.1296940	-2.2196273	1.9537623
C	2.6115444	-4.7039337	0.7721179
H	3.0951307	-3.2311928	-0.7299918
C	1.8037527	-5.0294845	1.8636239
H	0.1850636	-4.3777951	3.1456449
H	3.3731101	-5.4048769	0.4264803
H	1.9359413	-5.9838697	2.3760855
C	1.9326386	0.2935674	0.8253673
C	2.3891390	-0.0655995	2.1029864
C	1.9581765	1.6383018	0.4068627
C	2.8643478	0.9132545	2.9713890
H	2.3816398	-1.1079262	2.4168881
C	2.4258259	2.6178212	1.3169458
C	2.8763436	2.2536140	2.5924105
H	3.2267045	0.6312446	3.9612128
H	3.2362917	3.0082718	3.2894718
O	2.3769647	3.9002087	0.8710063
O	3.8287046	2.4777358	-1.3526739
C	2.8341949	4.9351634	1.7413069
H	2.7050285	5.8687223	1.1830649
H	2.2343563	4.9737390	2.6655193
H	3.8983561	4.8045028	1.9962266
C	4.8955507	2.9142585	-2.1942815
H	5.8120132	2.7542326	-1.6158034
H	4.9394155	2.3208996	-3.1222920
H	4.8010698	3.9840307	-2.4416022
C	-2.8322069	-5.2299538	1.3924593
C	-3.7874226	-4.3375831	1.7804620
C	-2.7657678	-3.4942131	-0.0395152
N	-2.2212210	-4.6983747	0.2717651
H	-2.5491368	-6.1911237	1.8041408
H	-4.5057394	-4.3764375	2.5901522
N	-3.7343855	-3.2807150	0.8876886
C	-4.5704628	-2.0748091	0.9594335
H	-5.5511081	-2.3892189	1.3463603
H	-4.7239578	-1.7223294	-0.0665864
C	-3.9806390	-0.9740196	1.8168796
H	-3.8647019	-0.0040764	1.3263122
C	-3.6321148	-1.1191053	3.0965733
H	-3.7289602	-2.0693162	3.6276609
H	-3.2263952	-0.2819042	3.6647831
C	-1.1485066	-5.3273321	-0.4912172
B	-2.3415317	-2.5916788	-1.2747317
H	-2.7504861	-3.0436096	-2.3249618
H	-2.7608455	-1.3898138	-1.1534392
H	-1.0463827	-2.6039422	-1.4072120
H	-0.2363620	-4.7205657	-0.4264481
H	-0.9523326	-6.3192395	-0.0719224
H	-1.4489856	-5.4248278	-1.5418915

TsI_IIR.xyz
98
Energy = -2817.826371612
Rh -0.9267181 -1.2251794 -0.2330337
P   1.3441638 -1.2003148 -0.1354729
P   -0.9678903   1.0954230 -0.2205784
C   -2.4923733   1.6143684 -1.1107684
C   -3.4331202   2.4927174 -0.5584700
C   -2.7528980   1.0392112 -2.3676266
C   -4.6061288   2.7985413 -1.2554099
H   -3.2612348   2.9344922   0.4229715
C   -3.9154554   1.3577597 -3.0668516
H   -2.0396687   0.3291133 -2.7920266
C   -4.8482427   2.2387411 -2.5100489
H   -5.3317984   3.4819369 -0.8111168
H   -4.0978744   0.9127269 -4.0465464
H   -5.7621170   2.4840247 -3.0534359
C   0.3987693   1.9550349 -1.1025405
C   1.6888812   1.9281900 -0.5386456
C   0.1832359   2.5618472 -2.3493381
C   2.7600512   2.5041436 -1.2652793
C   1.2491244   3.1350879 -3.0380653
H   -0.8173276   2.6018105 -2.7758810
C   2.5382516   3.1036539 -2.5110020
H   1.0747205   3.6141794 -4.0028447
H   3.3617051   3.5451126 -3.0693913
C   -1.0296489   1.9973226   1.3781595
C   -0.9045658   3.3968598   1.3988609
C   -1.1954262   1.3043825   2.5840405
C   -0.9639320   4.0886804   2.6084372
H   -0.7455719   3.9443891   0.4681758
C   -1.2394683   1.9985422   3.7940077
H   -1.2785701   0.2176787   2.5734338
C   -1.1286023   3.3908054   3.8085503
H   -0.8726476   5.1762985   2.6136498
H   -1.3567471   1.4486559   4.7292427
H   -1.1680319   3.9330140   4.7549252
C   2.3818212 -0.8284070 -1.6018232
C   3.7783329 -0.7537555 -1.4617177
C   1.8044354 -0.6038196 -2.8583863
C   4.5807810 -0.4917722 -2.5716356
H   4.2368629 -0.8857803 -0.4800143
C   2.6096486 -0.3309312 -3.9645082
H   0.7183473 -0.6036782 -2.9545662
C   3.9984774 -0.2839494 -3.8254529
H   5.6647535 -0.4425496 -2.4544966
H   2.1490944 -0.1437948 -4.9356475
H   4.6279767 -0.0765043 -4.6923902
C   1.9354120 -2.8491826   0.4384499
C   1.3232490 -3.4121056   1.5761110
C   2.8810101 -3.6107772 -0.2622791
C   1.6839911 -4.6812003   2.0242317
H   0.5379502 -2.8589513   2.0960633
C   3.2294141 -4.8904992   0.1810305
H   3.3468781 -3.2139722 -1.1637602
C   2.6426388 -5.4244628   1.3279636
H   1.2087804 -5.0952423   2.9151549
H   3.9653103 -5.4698707 -0.3787828
H   2.9215248 -6.4207964   1.6742780
C   1.9526181 -0.0000529   1.1274283
C   2.2983581 -0.4382614   2.4154968
C   1.9770140   1.3753161   0.8166472
C   2.6512522   0.4829796   3.3974661
H   2.3165497 -1.4998045   2.6512667
C   2.3343592   2.2939214   1.8360462
C   2.6621292   1.8477806   3.1218556
H   2.9244319   0.1327730   4.3940996
H   2.9302747   2.5557661   3.9038792
O   2.3156424   3.6031462   1.4750261
O   3.9818917   2.4092693 -0.6781672
C   2.6628991   4.5792695   2.4563118
H   2.5823042   5.5474680   1.9502105
H   1.9652337   4.5528025   3.3093614
H   3.6951914   4.4380552   2.8154308
C   5.1013065   2.9768725 -1.3569868
H   5.9649650   2.7910820 -0.7092214
H   5.2639118   2.4913612 -2.3333314
H   4.9762778   4.0625289 -1.4994894
C   -5.6638964 -3.9886019   0.7535757
C   -4.6796510 -4.6512447   0.0836488
C   -3.8598422 -2.6409553   0.6652455
N   -5.1460392 -2.7571928   1.1012699
H   -6.6740070 -4.2872626   1.0073869
H   -4.6661653 -5.6416152 -0.3560202
N   -3.5818800 -3.8100196   0.0392656
C   -2.3093756 -4.2745293 -0.5737078
H   -2.6050769 -4.6922937 -1.5490787
H   -1.9864898 -5.1206483   0.0506548
C   -1.1067574 -3.3670420 -0.7683109
H   -0.2190176 -3.8494343 -0.3584824
C   -0.8877634 -2.5559348 -1.9121951
H   -1.7191264 -2.3287176 -2.5879674
H   0.0876630 -2.5804958 -2.3996279
C   -5.8859571 -1.7138781   1.8068419
B   -2.9606411 -1.3566430   0.7878463
H   -3.5658067 -0.4025422   1.2116728
H   -1.9058089 -1.5797210   1.4552691
H   -2.6825541 -1.0673610 -0.4546582
H   -6.0078038 -0.8338430   1.1638139
H   -6.8701175 -2.1115527   2.0766551
H   -5.3500296 -1.4179924   2.7156693

TsII_IIIR.xyz
98
Energy = -2817.814902887

Rh	-1.3263971	0.1598186	0.5559311
H	-2.4232048	0.4611281	-1.7371843
H	-2.3980510	-0.9227128	0.9233367
B	-2.9121667	-0.3179932	-0.9378435
H	-2.9460617	-1.4706577	-1.3013339
C	-6.4569286	0.4295681	0.2048385
C	-5.8430839	1.6277837	0.4303507
H	-7.4829294	0.1190235	0.3625420
H	-6.2277511	2.5556220	0.8368710
C	-4.3008111	0.2192788	-0.4241919
N	-4.5298572	1.4822145	0.0336609
N	-5.4964336	-0.4226829	-0.3091938
C	-2.4046265	2.0513362	1.1711571
C	-2.5822432	1.0300536	2.1060550
H	-3.5409933	0.5209864	2.2046207
H	-1.9564984	0.9987839	3.0020075
H	-1.6594855	2.8269306	1.3578244
P	-0.1457212	-1.7552969	0.1409616
P	0.4536774	1.6414713	-0.1858230
C	1.3725373	-1.5023375	1.1577994
C	2.4069626	-0.6606157	0.6911960
C	1.4079674	-2.0055415	2.4689637
C	3.4558386	-0.3256706	1.5849614
C	2.4543907	-1.6679679	3.3223479
H	0.6238698	-2.6743214	2.8192785
C	3.4735699	-0.8203093	2.8951162
H	2.4779335	-2.0703908	4.3363518
H	4.2801651	-0.5566732	3.5768827
C	1.7914437	0.9322065	-1.2250543
C	2.0596947	1.4281006	-2.5101195
C	2.5326868	-0.1480239	-0.7091239
C	3.0499242	0.8410507	-3.2921788
H	1.5052313	2.2801230	-2.8985912
C	3.5363090	-0.7266581	-1.5243440
C	3.7847719	-0.2406539	-2.8131685
H	3.2548226	1.2314257	-4.2902705
H	4.5505650	-0.6941395	-3.4398530
C	-3.4700722	2.4776611	0.1846964
H	-3.9478554	3.4120706	0.5184482
H	-3.0253893	2.6734712	-0.8026175
C	0.4560281	-2.2647805	-1.5089242
C	1.4611329	-3.2412555	-1.6163945
C	-0.1066693	-1.7197648	-2.6699179
C	1.8862401	-3.6704603	-2.8729088
H	1.9232044	-3.6515934	-0.7168367
C	0.3322861	-2.1440925	-3.9253514
H	-0.8887362	-0.9648803	-2.5862754
C	1.3242380	-3.1214489	-4.0291930
H	2.6618263	-4.4346401	-2.9490245
H	-0.1047833	-1.7098685	-4.8259156
H	1.6617182	-3.4553671	-5.0117458
C	-0.9705366	-3.2707166	0.7975593
C	-1.6675386	-3.1895846	2.0170775
C	-0.9718706	-4.4892918	0.1044738
C	-2.3178439	-4.3044702	2.5434734
H	-1.7112262	-2.2381175	2.5504429
C	-1.6407155	-5.6011466	0.6249133
H	-0.4650662	-4.5774585	-0.8555628
C	-2.3072495	-5.5164672	1.8469459
H	-2.8415479	-4.2237806	3.4975685
H	-1.6382006	-6.5377930	0.0650559
H	-2.8237906	-6.3876073	2.2529779
C	-0.2383516	3.0279666	-1.1651759
C	-0.2779608	4.3422199	-0.6738276
C	-0.8879423	2.7386169	-2.3802347
C	-0.9448358	5.3441804	-1.3843700
H	0.2166081	4.5894073	0.2665420
C	-1.5398162	3.7448115	-3.0934838
H	-0.8881917	1.7193126	-2.7684438
C	-1.5737170	5.0509243	-2.5958052
H	-0.9630540	6.3614356	-0.9896764
H	-2.0283807	3.5046376	-4.0392683
H	-2.0862304	5.8367813	-3.1526014
C	1.3984526	2.4397515	1.1689445
C	2.5005692	3.2641969	0.8885942
C	1.0468280	2.1950762	2.5029764
C	3.2172358	3.8534685	1.9292832
H	2.8029876	3.4350602	-0.1463733
C	1.7709813	2.7778363	3.5447926
H	0.2203818	1.5173865	2.7259213
C	2.8526453	3.6130646	3.2583326
H	4.0694072	4.4967069	1.7033198
H	1.4942090	2.5727026	4.5800197
H	3.4176443	4.0733205	4.0707189
O	4.4110659	0.4978197	1.0786896
O	4.2069311	-1.7720045	-0.9695699
C	5.2552487	-2.3770143	-1.7259223
H	5.6575623	-3.1727571	-1.0895691
H	4.8725378	-2.8143905	-2.6627266
H	6.0527568	-1.6522473	-1.9565891
C	5.4880896	0.8898453	1.9292353
H	6.1201149	1.5449908	1.3198703
H	5.1215081	1.4490762	2.8053249
H	6.0759511	0.0188173	2.2613029
C	-5.7469347	-1.8071895	-0.6956218
H	-6.2282141	-1.8477828	-1.6819607
H	-4.7907860	-2.3373893	-0.7389789
H	-6.3998191	-2.2767145	0.0498494

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TsIII_IVR.xyz
98
Energy = -2817.807762450
Rh  -1.2800227   0.1284238   0.6750147
H   -2.2874440   0.3836012  -1.8353805
H   -2.2967059  -0.8165762   1.5204802
B   -2.6725558  -0.3958200  -0.9882349
H   -2.5713489  -1.5647958  -1.2833061
C   -6.3483701  -0.1027637  -0.0995605
C   -5.8920448   1.1250738   0.2867553
H   -7.3442541  -0.5286881  -0.0724796
H   -6.4099548   1.9650408   0.7342713
C   -4.1347809  -0.0307872  -0.5290145
N   -4.5413912   1.1522653   0.0082319
N   -5.2577469  -0.8008918  -0.5843802
C   -2.5804580   1.7067231   1.3990919
C   -2.8171359   0.5230832   2.1720434
H   -3.8116526   0.0649784   2.1583178
H   -2.3448695   0.4558629   3.1574183
H   -1.9919861   2.5090395   1.8502969
P   -0.0233416  -1.7402120   0.1990748
P    0.2503502   1.6605600  -0.2340018
C    1.5198754  -1.3769011   1.1426596
C    2.4519424  -0.4574083   0.6097561
C    1.6764275  -1.8672413   2.4492035
C    3.5272125  -0.0391277   1.4348118
C    2.7438766  -1.4425346   3.2351854
H    0.9743290  -2.5982645   2.8462689
C    3.6644590  -0.5207134   2.7426443
H    2.8634812  -1.8355170   4.2461666
H    4.4883614  -0.1894928   3.3721348
C    1.6136579   1.0556186  -1.3035154
C    1.7886690   1.5485049  -2.6054560
C    2.4600468   0.0453300  -0.8020495
C    2.7870635   1.0268170  -3.4226493
H    1.1573339   2.3522040  -2.9787808
C    3.4683981  -0.4684810  -1.6561936
C    3.6210978   0.0115930  -2.9621509
H    2.9190053   1.4157082  -4.4335348
H    4.3901424  -0.3949847  -3.6163484
C   -3.6041206   2.2076962   0.3951657
H   -4.2039032   3.0302782   0.8153110
H   -3.1110327   2.5909473  -0.5110139
O    4.3860184   0.8491651   0.8676745
O    4.2441789  -1.4469993  -1.1186373
C    5.4923651   1.3102424   1.6417745
H    6.0395005   2.0008005   0.9906802
H    5.1536237   1.8487207   2.5419272
H    6.1542151   0.4783502   1.9324013
C    5.2923487  -1.9922297  -1.9188497
H    5.7828589  -2.7437411  -1.2906486
H    4.8929048  -2.4760014  -2.8253238
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H    6.0230562  -1.2181754  -2.2043574
C   -5.3149683  -2.1577897  -1.1203365
H   -5.3797420  -2.1360488  -2.2160201
H   -4.4095396  -2.7000494  -0.8283568
H   -6.1987005  -2.6598775  -0.7112345
C   -0.5385434   3.0571364  -1.1195351
C   -0.6680035   4.3186560  -0.5150986
C   -1.1809445   2.8303406  -2.3517200
C   -1.4069995   5.3298906  -1.1337054
H   -0.1875915   4.5167703   0.4435707
C   -1.9088326   3.8472534  -2.9713134
H   -1.1212618   1.8513855  -2.8271875
C   -2.0257226   5.1002725  -2.3642084
H   -1.4909887   6.3052354  -0.6514641
H   -2.3901814   3.6553744  -3.9316742
H   -2.5958681   5.8940640  -2.8490948
C    1.1723253   2.4542329   1.1435191
C    0.8525307   2.1609036   2.4764833
C    2.2275564   3.3399637   0.8715011
C    1.5635566   2.7496217   3.5233626
H    0.0585998   1.4431257   2.6979019
C    2.9285681   3.9386743   1.9177093
H    2.5054049   3.5535445  -0.1623164
C    2.5981625   3.6451668   3.2445951
H    1.3135016   2.5031541   4.5563141
H    3.7425009   4.6311888   1.6964918
H    3.1514942   4.1119372   4.0612456
C   -0.7479947  -3.2925786   0.8897591
C   -0.8246558  -4.4809649   0.1489793
C   -1.3278104  -3.2659770   2.1711841
C   -1.4485048  -5.6133432   0.6818209
H   -0.4085106  -4.5289037  -0.8564676
C   -1.9287538  -4.4016747   2.7110544
H   -1.3189882  -2.3409168   2.7509422
C   -1.9927872  -5.5824785   1.9651699
H   -1.5047743  -6.5245191   0.0838959
H   -2.3567915  -4.3618690   3.7141957
H   -2.4719040  -6.4698402   2.3816879
C    0.5976582  -2.2630997  -1.4456139
C    0.0672433  -1.7424771  -2.6327275
C    1.6213121  -3.2246807  -1.5096322
C    0.5524825  -2.1782186  -3.8669288
H   -0.7204718  -0.9920393  -2.5887000
C    2.0921771  -3.6673966  -2.7450351
H    2.0593954  -3.6178290  -0.5904814
C    1.5596741  -3.1436299  -3.9265403
H    0.1411564  -1.7589977  -4.7865716
H    2.8808769  -4.4208637  -2.7839663
H    1.9319512  -3.4870727  -4.8932114
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TsIV_VR.xyz
98
Energy = -2817.821604328

Rh	-0.3703105	1.5422601	0.3906698
H	2.3952015	1.2910961	1.0605786
H	-0.9688263	3.7498269	-0.0718973
B	1.5194750	2.1322788	1.1511192
H	1.5577781	2.9803002	0.2566787
C	2.4568401	3.7512482	4.4350481
C	1.1024332	3.7253734	4.5886507
H	3.2378012	4.1371989	5.0795434
H	0.4745430	4.0611600	5.4050242
C	1.5701084	2.7983837	2.5901868
N	0.5793458	3.1451746	3.4484749
N	2.7261200	3.1772074	3.2075228
C	-1.2895597	2.6976218	1.8445431
C	-1.1860768	3.9696967	1.0032428
H	-0.3682365	4.6250142	1.3334166
H	-2.1252449	4.5461512	0.9776574
H	-2.3287548	2.3271643	1.8793601
P	0.1675041	0.7703191	-1.7927056
P	-0.5412795	-0.4429932	1.2863407
C	-1.0766451	-0.5159056	-2.2264115
C	-0.9520621	-1.7738120	-1.6025168
C	-2.1718172	-0.2425956	-3.0586174
C	-1.9535028	-2.7472506	-1.8351871
C	-3.1489800	-1.2136094	-3.2655354
H	-2.2524548	0.7197222	-3.5617240
C	-3.0536658	-2.4613898	-2.6535399
H	-3.9964795	-0.9988456	-3.9185613
H	-3.8281064	-3.2072629	-2.8230994
C	0.5157452	-1.7428631	0.5181026
C	1.6337125	-2.2429509	1.2051592
C	0.2419704	-2.1770859	-0.7980807
C	2.4926225	-3.1474027	0.5883881
H	1.8265267	-1.9479782	2.2332047
C	1.1302289	-3.1052894	-1.4003518
C	2.2563620	-3.5752310	-0.7149311
H	3.3582370	-3.5289580	1.1321458
H	2.9423779	-4.2754728	-1.1879573
C	-0.8496484	2.8350250	3.2809836
H	-1.3938173	3.6492703	3.7927446
H	-1.0551618	1.9057697	3.8324253
C	4.0521534	3.0272042	2.6197744
H	4.2673332	1.9656558	2.4434599
H	4.1022298	3.5590919	1.6614641
H	4.7929701	3.4446553	3.3098612
C	1.7335514	0.0724555	-2.4375519
C	1.7544759	-0.6024711	-3.6693885
C	2.9245921	0.2402159	-1.7191567
C	2.9566181	-1.0970648	-4.1743723
H	0.8281140	-0.7485238	-4.2275454

C	4.1237075	-0.2664232	-2.2244980
H	2.9053338	0.7573712	-0.7601504
C	4.1424133	-0.9336281	-3.4511559
H	2.9674679	-1.6136380	-5.1359067
H	5.0470203	-0.1398733	-1.6566328
H	5.0813717	-1.3243235	-3.8472344
C	-0.1719936	2.1903672	-2.9115011
C	-1.3618902	2.9211034	-2.7299313
C	0.7539971	2.6384403	-3.8644119
C	-1.6283727	4.0545787	-3.4962150
H	-2.0945420	2.5945984	-1.9865492
C	0.4914285	3.7836209	-4.6214284
H	1.6874683	2.0961932	-4.0157327
C	-0.6980857	4.4912728	-4.4442423
H	-2.5616948	4.6008349	-3.3500643
H	1.2243138	4.1210517	-5.3561282
H	-0.9006661	5.3824690	-5.0399848
C	-2.2369691	-1.1282637	1.1346670
C	-2.4867595	-2.4648801	1.4867091
C	-3.2953110	-0.3252977	0.6880454
C	-3.7807029	-2.9783061	1.4065917
H	-1.6664581	-3.1057963	1.8144544
C	-4.5858555	-0.8467187	0.5919248
H	-3.1031940	0.7093457	0.3969844
C	-4.8308798	-2.1724890	0.9566224
H	-3.9682507	-4.0150466	1.6913532
H	-5.4001839	-0.2177610	0.2295426
H	-5.8411447	-2.5794031	0.8891054
C	-0.2098998	-0.5082635	3.0988318
C	-1.2321419	-0.7982072	4.0173005
C	1.0550956	-0.1418889	3.5951402
C	-0.9915294	-0.7334077	5.3926310
H	-2.2265434	-1.0693394	3.6639524
C	1.2945521	-0.0888322	4.9677427
H	1.8526624	0.1209471	2.9004014
C	0.2705466	-0.3817460	5.8729157
H	-1.7998830	-0.9609690	6.0893603
H	2.2846958	0.1912582	5.3316827
H	0.4564045	-0.3350261	6.9469906
O	0.8137002	-3.4767411	-2.6680910
O	-1.7675929	-3.9397251	-1.2081795
C	-2.7127865	-4.9812535	-1.4482675
H	-2.3543033	-5.8436577	-0.8755439
H	-3.7183002	-4.6994765	-1.0946865
H	-2.7570202	-5.2431172	-2.5177454
C	1.6592495	-4.4184056	-3.3277966
H	1.2076257	-4.5798264	-4.3126943
H	2.6788188	-4.0189019	-3.4538065
H	1.6987396	-5.3744044	-2.7810113

TsV_VIR.xyz
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Energy = -2817.811676430

Rh	-1.2776399	-0.2423866	0.1911438
H	-2.8597237	-0.5271446	-1.7295509
H	-2.3788431	-0.0540383	2.8863750
B	-3.1514919	-0.6128365	-0.5458640
H	-2.5775566	-1.5707111	0.1094034
C	-6.9406085	-0.5327320	-0.4723688
C	-6.5770097	0.6878098	0.0278911
H	-7.9196438	-0.9558707	-0.6645606
H	-7.1784861	1.5329742	0.3404388
C	-4.7042869	-0.4844153	-0.3597291
N	-5.1995329	0.6851758	0.0884472
N	-5.7713632	-1.2384628	-0.7145099
C	-2.9913248	0.9889021	1.0741170
C	-3.3008293	0.2888844	2.3970985
H	-3.9418934	-0.5960231	2.2669610
H	-3.8142397	0.9715290	3.0997845
H	-2.2768417	1.8040882	1.2566605
P	0.4888278	-1.6651509	0.2148610
P	0.0519045	1.5190734	-0.1380900
C	1.9548204	-1.0357525	1.1259186
C	2.7308052	-0.0083042	0.5525994
C	2.2111123	-1.4756964	2.4335819
C	3.7599170	0.5748164	1.3320866
C	3.2326752	-0.8909249	3.1769454
H	1.6183677	-2.2795430	2.8675236
C	4.0043085	0.1372081	2.6398669
H	3.4324149	-1.2391832	4.1915647
H	4.7928600	0.5899590	3.2382542
C	1.4648296	1.2498301	-1.2833522
C	1.4074581	1.7214825	-2.6040021
C	2.5586280	0.4721496	-0.8513668
C	2.4257117	1.4111621	-3.5007587
H	0.5759217	2.3426580	-2.9309027
C	3.5776149	0.1632405	-1.7858286
C	3.5064803	0.6266814	-3.1052750
H	2.3782574	1.7846162	-4.5248818
H	4.2891385	0.3842477	-3.8218633
C	-4.2237582	1.6975147	0.5156444
H	-4.7070736	2.3219747	1.2858224
H	-3.9713412	2.3366760	-0.3438610
C	-5.6857144	-2.5990467	-1.2315865
H	-4.6885592	-2.7487791	-1.6612145
H	-5.8466330	-3.3287751	-0.4267322
H	-6.4413983	-2.7427394	-2.0127757
C	-0.0198700	-3.1893149	1.1103078
C	0.2947308	-4.4821720	0.6686246
C	-0.7950940	-3.0361047	2.2735597
C	-0.1489430	-5.5974374	1.3840766
H	0.8788577	-4.6251107	-0.2405557
C	-1.2262672	-4.1503587	2.9920580
H	-1.0630984	-2.0311672	2.6084997
C	-0.9042005	-5.4358190	2.5469364
H	0.0995535	-6.5984375	1.0275382
H	-1.8194307	-4.0151224	3.8980879
H	-1.2458586	-6.3098208	3.1037755
C	1.1473907	-2.2602160	-1.3846504
C	2.3763071	-2.9361130	-1.4563561
C	0.3984545	-2.0579667	-2.5519310
C	2.8401020	-3.4115491	-2.6829818
H	2.9788156	-3.0714627	-0.5564426
C	0.8718955	-2.5257993	-3.7785590
H	-0.5479489	-1.5157472	-2.4886793
C	2.0908326	-3.2050206	-3.8451104
H	3.7929940	-3.9416767	-2.7320424
H	0.2898353	-2.3557669	-4.6857612
H	2.4595934	-3.5723663	-4.8043010
C	0.8194532	2.3253535	1.3174838
C	1.7790691	3.3385020	1.1559160
C	0.4349245	1.9373171	2.6079890
C	2.3298873	3.9623911	2.2749955
H	2.1057021	3.6270030	0.1551691
C	0.9974130	2.5553166	3.7257233
H	-0.2879393	1.1268202	2.7244354
C	1.9416663	3.5711598	3.5603506
H	3.0702541	4.7534973	2.1432051
H	0.7025970	2.2384638	4.7273002
H	2.3794920	4.0572301	4.4338668
C	-0.9655946	2.8442255	-0.9176839
C	-1.0645729	4.1376413	-0.3857265
C	-1.7450802	2.5103006	-2.0405850
C	-1.9162803	5.0798979	-0.9714556
H	-0.4827925	4.4151824	0.4933880
C	-2.5772099	3.4580745	-2.6349018
H	-1.7102198	1.4933590	-2.4356965
C	-2.6674430	4.7473017	-2.0991284
H	-1.9863845	6.0805138	-0.5417326
H	-3.1634434	3.1868058	-3.5147245
H	-3.3245173	5.4873964	-2.5585929
O	4.4530702	1.5770744	0.7292202
O	4.5879046	-0.6139700	-1.3130121
C	5.6522075	-0.9503603	-2.2021378
H	6.3431080	-1.5661687	-1.6160209
H	5.2846743	-1.5306542	-3.0644966
H	6.1768342	-0.0494260	-2.5595043
C	5.5049285	2.2040955	1.4616587
H	5.9187044	2.9652957	0.7911752
H	5.1220702	2.6887710	2.3749109
H	6.2940725	1.4826237	1.7286660

Ts0_IS.xyz
98
Energy = -2817.813326731

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Rh  -1.3395639   0.5588740  -0.3145181
P   -0.2585004  -1.2917597   0.0506545
P    0.5677161   1.7219159  -0.3506499
C    0.1456049   3.2831862  -1.2254804
C    0.5224765   4.5537482  -0.7661230
C   -0.6925164   3.1858930  -2.3531670
C    0.0765729   5.7015821  -1.4257571
H    1.1562808   4.6534443   0.1152964
C   -1.1301508   4.3342304  -3.0123802
H   -1.0085484   2.2003319  -2.7056987
C   -0.7474355   5.5960625  -2.5484321
H    0.3758938   6.6841145  -1.0571554
H   -1.7752212   4.2423611  -3.8876795
H   -1.0930586   6.4956887  -3.0600522
C    1.8655413   0.9123190  -1.3701204
C    2.5594551  -0.1911642  -0.8356744
C    2.0759376   1.3091323  -2.6991428
C    3.4535827  -0.8996921  -1.6744912
C    2.9667384   0.6018325  -3.5020050
H    1.5524114   2.1733751  -3.1045391
C    3.6511195  -0.5049814  -3.0035592
H    3.1317179   0.9150839  -4.5340960
H    4.3359061  -1.0518674  -3.6491614
C    1.4659964   2.2440602   1.1599395
C    2.7254200   2.8604855   1.0777365
C    0.8880355   2.0216913   2.4172930
C    3.3802787   3.2695767   2.2394851
H    3.2006354   3.0034501   0.1053824
C    1.5506246   2.4214365   3.5784916
H   -0.0705638   1.5002399   2.4735657
C    2.7941702   3.0517004   3.4902927
H    4.3553107   3.7549355   2.1683838
H    1.1003598   2.2322777   4.5542217
H    3.3113191   3.3682807   4.3976025
C    0.2761536  -2.2590012  -1.4106691
C    1.1599330  -3.3425119  -1.2723029
C   -0.2164598  -1.9245483  -2.6797494
C    1.5307462  -4.0877072  -2.3916762
H    1.5766734  -3.5880077  -0.2938348
C    0.1669039  -2.6661809  -3.7979936
H   -0.8854451  -1.0669233  -2.7793569
C    1.0374253  -3.7494923  -3.6553044
H    2.2146092  -4.9306739  -2.2772122
H   -0.2114158  -2.3935548  -4.7844429
H    1.3358550  -4.3292927  -4.5304197
C   -1.3953962  -2.4195805   0.9711010
C   -2.1945160  -1.8601768   1.9837262
C   -1.5199065  -3.7866063   0.6863073
C   -3.0845287  -2.6522204   2.7084629
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H   -2.1137955  -0.7892498   2.1879028
C   -2.4183234  -4.5782280   1.4084834
H   -0.9230163  -4.2382768  -0.1063158
C   -3.1991464  -4.0162566   2.4210756
H   -3.6936404  -2.2034806   3.4951691
H   -2.5055213  -5.6409553   1.1761031
H   -3.8954725  -4.6392375   2.9849523
C    1.2465399  -1.2114179   1.1019297
C    1.1899590  -1.6263593   2.4421766
C    2.4195365  -0.6258992   0.5848021
C    2.2966596  -1.4582526   3.2697321
H    0.2872504  -2.0900632   2.8365386
C    3.5255607  -0.4479959   1.4523817
C    3.4618017  -0.8653514   2.7880025
H    2.2527546  -1.7906050   4.3081309
H    4.3124873  -0.7281654   3.4531489
O    4.6054430   0.1663791   0.9037266
O    4.0643856  -1.9725295  -1.1049419
C    5.7533980   0.3748999   1.7258902
H    6.4905785   0.8687173   1.0835008
H    5.5170860   1.0274691   2.5824437
H    6.1656627  -0.5800447   2.0899778
C    4.9826002  -2.7239216  -1.8980306
H    5.3510332  -3.5233594  -1.2458280
H    4.4832088  -3.1669824  -2.7753168
H    5.8296406  -2.1017232  -2.2295151
C   -6.1488723  -1.0762027   1.2167684
C   -5.9902758   0.2070794   1.6496671
C   -4.6225551  -0.0925651  -0.1193867
N   -5.3092394  -1.2384554   0.1299955
H   -6.7847314  -1.8740647   1.5807920
H   -6.4722131   0.7500922   2.4539475
N   -5.0520877   0.7918303   0.8183675
C   -4.5610555   2.1681385   0.9230499
H   -5.2516511   2.6951383   1.5996400
H   -4.6366289   2.6434645  -0.0647743
C   -3.1571119   2.2699204   1.4499258
H   -2.9182970   1.6596167   2.3264977
C   -2.2739274   3.1643019   0.9812551
H   -2.5054178   3.8016256   0.1248878
H   -1.3142613   3.3268818   1.4684907
C   -5.1172922  -2.4885984  -0.5954907
B   -3.5125932   0.1306460  -1.2247471
H   -3.8082904  -0.3993203  -2.2762027
H   -3.2098752   1.3119886  -1.3770480
H   -2.5152162  -0.6285135  -0.8929276
H   -4.2949574  -3.0617373  -0.1458306
H   -6.0422797  -3.0740880  -0.5505554
H   -4.8725418  -2.2613288  -1.6382127
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Ts0_IIS.xyz
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Rh	-0.9535348	-0.9199743	-0.2173308
P	1.2232871	-0.9285512	-0.0998332
P	-0.9903889	1.3096282	-0.1223800
C	-2.6041486	1.8503875	-0.8191199
C	-3.5085308	2.6575217	-0.1135195
C	-2.9685907	1.3657469	-2.0892147
H	-3.2521036	3.0299217	0.8786364
C	-4.7441068	2.9892876	-0.6762345
H	-2.2890053	0.7014606	-2.6280869
C	-5.0852277	2.5292022	-1.9497339
H	-5.4394424	3.6165843	-0.1159879
H	-4.4564703	1.3461619	-3.6484154
H	-6.0469773	2.7982328	-2.3892274
C	0.2815649	2.2291809	-1.0778424
C	1.6154797	2.1975238	-0.6263255
C	-0.0423082	2.8456426	-2.2958219
C	2.6195077	2.7651824	-1.4495724
C	0.9595387	3.4139148	-3.0771772
H	-1.0767184	2.8939333	-2.6304276
C	2.2910275	3.3660223	-2.6705566
H	0.7021754	3.8986355	-4.0202130
H	3.0644157	3.8009760	-3.3010123
C	-0.9202203	2.0774835	1.5421005
C	-0.8000025	3.4684537	1.6917558
C	-0.9897791	1.2648920	2.6816374
C	-0.7642053	4.0330252	2.9669814
H	-0.7147076	4.1070904	0.8106476
C	-0.9431755	1.8311621	3.9560536
H	-1.0438507	0.1808548	2.5485083
C	-0.8340432	3.2164931	4.0999277
H	-0.6737962	5.1151978	3.0768488
H	-0.9818441	1.1904241	4.8385680
H	-0.7977927	3.6608536	5.0960002
C	2.0642990	-0.6712432	-1.7069812
C	3.4491131	-0.4419368	-1.7553976
C	1.3299588	-0.7412984	-2.8982532
C	4.0862414	-0.2869000	-2.9864001
H	4.0247058	-0.3675766	-0.8311550
C	1.9700815	-0.5715455	-4.1265688
H	0.2528083	-0.9174931	-2.8449087
C	3.3478293	-0.3455374	-4.1721890
H	5.1634511	-0.1141931	-3.0190484
H	1.3910698	-0.6149142	-5.0503873
H	3.8479670	-0.2148614	-5.1333132
C	1.8085398	-2.5831161	0.4633549
C	1.2744454	-3.1308876	1.6437331
C	2.7080335	-3.3477970	-0.2910276
C	1.6527042	-4.4011939	2.0723075

H	0.5445160	-2.5584018	2.2205501
C	3.0733298	-4.6292555	0.1324757
H	3.1184802	-2.9543619	-1.2204886
C	2.5534830	-5.1568103	1.3140319
H	1.2389793	-4.8072799	2.9969990
H	3.7679740	-5.2155070	-0.4713195
H	2.8433906	-6.1559869	1.6429735
C	2.0226638	0.2806194	1.0313252
C	2.5057644	-0.1484109	2.2786774
C	2.0281573	1.6519075	0.7011304
C	2.9753151	0.7777478	3.2044867
H	2.5330778	-1.2085473	2.5214851
C	2.4901311	2.5769754	1.6714734
C	2.9572584	2.1405010	2.9170522
H	3.3586412	0.4353480	4.1670066
H	3.3118977	2.8542107	3.6583932
O	2.4237762	3.8853886	1.3095651
O	3.8906663	2.6597194	-0.9783599
C	2.8817863	4.8662947	2.2393954
H	2.7416733	5.8323396	1.7423249
H	2.2897099	4.8427493	3.1691963
H	3.9489919	4.7274174	2.4768698
C	4.9477525	3.2129289	-1.7613840
H	5.8668634	3.0140420	-1.1994444
H	5.0094073	2.7278934	-2.7494865
H	4.8251560	4.3004838	-1.8910904
C	-4.1332933	-5.5522889	0.6267827
C	-4.3222979	-4.5075824	1.4809175
C	-2.7388520	-3.8942615	-0.0114500
N	-3.1604587	-5.1618873	-0.2743732
H	-4.6019318	-6.5282285	0.5874103
H	-4.9909172	-4.3938675	2.3257341
N	-3.4571059	-3.5043997	1.0836700
C	-3.2972968	-2.2367120	1.7903220
H	-2.2173855	-2.0768717	1.9643049
H	-3.7681740	-2.3546697	2.7788904
C	-3.8639511	-1.0332607	1.0876803
H	-3.6964431	-0.0924410	1.6205367
C	-4.5388554	-1.0356724	-0.0647238
H	-4.7228400	-1.9532471	-0.6263209
H	-4.9198209	-0.1089832	-0.4924297
C	-2.6180402	-6.0156875	-1.3282389
B	-1.6534590	-3.0809229	-0.8260889
H	-1.0275078	-3.7875614	-1.5794206
H	-2.1570594	-2.1221755	-1.4494470
H	-0.8293473	-2.6799292	0.0771333
H	-1.5524938	-6.2021281	-1.1468767
H	-3.1636865	-6.9651973	-1.3198145
H	-2.7319378	-5.5326908	-2.3049629

TsI_IIS.xyz
98
Energy = -2817.813667560

Rh	-0.9239923	-1.2463406	0.6474607
P	1.3226055	-1.1131458	0.3388530
P	-1.0952678	0.9863348	0.3850503
C	-2.8210487	1.2571579	-0.1966342
C	-3.7051297	2.1483923	0.4281533
C	-3.2985572	0.4498870	-1.2460550
H	-3.3643680	2.7697338	1.2563260
C	-4.6204549	0.5544244	-1.6757589
H	-2.6262830	-0.2712118	-1.7149020
C	-5.4937353	1.4502726	-1.0516478
H	-5.7092722	2.9380135	0.4997645
H	-4.9727304	-0.0716698	-2.4973693
H	-6.5298674	1.5294230	-1.3843237
C	-0.0181882	1.6500296	-0.9550767
C	1.3577845	1.8133079	-0.6951686
C	-0.5334426	1.9158038	-2.2328293
C	2.2051167	2.2281225	-1.7516835
C	0.3185422	2.3312429	-3.2538731
H	-1.5993585	1.8194516	-2.4289669
C	1.6842097	2.4822464	-3.0271070
H	-0.0880248	2.5440829	-4.2439397
H	2.3357411	2.7984226	-3.8396573
C	-0.8427644	2.2090543	1.7288073
C	-0.9380666	3.5828493	1.4482166
C	-0.5255095	1.7951087	3.0285933
C	-0.7552838	4.5201684	2.4645083
H	-1.1418070	3.9196631	0.4299641
C	-0.3297703	2.7349558	4.0407999
H	-0.3864189	0.7339375	3.2333008
C	-0.4546305	4.0980328	3.7630418
H	-0.8381038	5.5846920	2.2388565
H	-0.0682544	2.4015395	5.0461363
H	-0.3087084	4.8332140	4.5562558
C	2.2769514	-1.1203501	-1.2310431
C	3.6690899	-0.9299315	-1.1783697
C	1.6555026	-1.3152915	-2.4697996
C	4.4241312	-0.9522310	-2.3501290
H	4.1615706	-0.7543460	-0.2202342
C	2.4136636	-1.3224542	-3.6420982
H	0.5765857	-1.4533108	-2.5140416
C	3.7975208	-1.1456130	-3.5851900
H	5.5049422	-0.8097352	-2.2988058
H	1.9192663	-1.4655956	-4.6043346
H	4.3896453	-1.1583247	-4.5019477
C	1.8719150	-2.6291634	1.2166986
C	1.3947867	-2.8698878	2.5198905
C	2.6553578	-3.6078258	0.5885459
C	1.7144363	-4.0525704	3.1841786

H	0.7670285	-2.1233558	3.0114198
C	2.9644987	-4.7964085	1.2547224
H	3.0212242	-3.4483703	-0.4257438
C	2.4999404	-5.0208892	2.5512860
H	1.3477949	-4.2203895	4.1982974
H	3.5733741	-5.5501740	0.7530572
H	2.7464079	-5.9492954	3.0686855
C	2.0848013	0.3084764	1.2241158
C	2.7262009	0.1422450	2.4604375
C	1.9644083	1.5889730	0.6485488
C	3.2377470	1.2519982	3.1302886
H	2.8475397	-0.8506424	2.8896050
C	2.4767502	2.7030874	1.3560411
C	3.1114726	2.5311027	2.5932811
H	3.7459733	1.1190709	4.0867147
H	3.5082382	3.3866439	3.1369058
O	2.2896143	3.9093367	0.7616377
O	3.5213511	2.3357235	-1.4376232
C	2.7766606	5.0735352	1.4283019
H	2.5198177	5.9157370	0.7766535
H	2.2877180	5.2054895	2.4074537
H	3.8698783	5.0328526	1.5608545
C	4.4320952	2.7256056	-2.4651711
H	5.4202661	2.7407041	-1.9926540
H	4.4332477	1.9976608	-3.2927516
H	4.1956332	3.7301183	-2.8517922
C	-4.9637477	-3.2172329	-2.0609196
C	-5.1189409	-3.1133514	-0.7124074
C	-2.9061132	-3.0771747	-1.1394028
N	-3.6024674	-3.1937713	-2.3046046
H	-5.6948319	-3.3012819	-2.8561499
H	-6.0120865	-3.0979850	-0.0997050
N	-3.8482792	-3.0227792	-0.1670922
C	-3.6075736	-3.0585563	1.2847553
H	-3.5063712	-4.1166726	1.5679997
H	-4.5348011	-2.6865408	1.7439560
C	-2.4187729	-2.3014818	1.8468098
H	-1.7454648	-2.9508845	2.4159036
C	-2.4472944	-0.9492357	2.2218093
H	-3.2912199	-0.3191647	1.9299310
H	-1.9200924	-0.6233140	3.1171577
C	-2.9767706	-3.2462863	-3.6190145
B	-1.3319585	-2.9113817	-1.1072462
H	-0.7607128	-3.8938486	-1.5472975
H	-1.0656971	-1.9675650	-1.8286933
H	-0.7916101	-2.9429831	0.0778500
H	-2.2328044	-4.0516466	-3.6459546
H	-3.7499596	-3.4309957	-4.3721557
H	-2.4689331	-2.2958141	-3.8327014

TsII_IIIS.xyz
98
Energy = -2817.806626670

Rh	-1.2871800	0.5296472	-0.2910907
H	-2.4437797	-0.5136917	-0.5476964
H	-2.5235694	1.4983334	1.5696702
B	-3.0827572	0.5607074	1.0204733
H	-3.2410894	-0.4299296	1.6815129
C	-6.4096934	1.0720943	-0.7213861
C	-5.7080112	2.1631201	-1.1504524
H	-7.4207144	0.7507344	-0.9420174
H	-5.9875981	2.9660762	-1.8222717
C	-4.3710769	0.9886077	0.2338868
N	-4.4682454	2.0947531	-0.5517706
N	-5.5742989	0.3611244	0.1197925
C	-2.1267904	2.3583423	-1.3387667
C	-2.1600700	1.2137202	-2.1437216
H	-3.1066779	0.7211976	-2.3728412
H	-1.3602677	1.0424205	-2.8701034
H	-1.3061243	3.0664026	-1.4643030
P	-0.4022951	-1.5436702	0.2874104
P	0.7882696	1.7129910	0.0333598
C	1.2842831	-1.6563153	1.0372395
C	2.3778776	-1.0545667	0.3812438
C	1.4803050	-2.3104783	2.2638903
C	3.6476007	-1.0845534	1.0043877
C	2.7435266	-2.3451858	2.8477628
H	0.6503667	-2.8067158	2.7617087
C	3.8291434	-1.7238817	2.2358841
H	2.8846088	-2.8606262	3.7990613
H	4.8061584	-1.7439312	2.7153752
C	1.7091750	0.7941224	-1.2584566
C	1.6099869	1.2552199	-2.5863069
C	2.2890027	-0.4580764	-0.9843799
C	2.1221446	0.4919739	-3.6293474
H	1.1305865	2.2105046	-2.8011277
C	2.8280909	-1.2054510	-2.0631670
C	2.7390894	-0.7334371	-3.3780376
H	2.0464460	0.8550379	-4.6555986
H	3.1382667	-1.3167512	-4.2057073
C	-3.3495856	3.0146179	-0.7395969
H	-3.1053615	3.4640909	0.2351571
H	-3.7056053	3.8257351	-1.3948985
C	-1.4707058	-2.5373347	1.4007426
C	-2.1723939	-3.6573708	0.9337223
C	-1.6878335	-2.1009208	2.7191391
C	-3.0593246	-4.3365388	1.7739428
H	-2.0273658	-4.0066436	-0.0890194
C	-2.5572454	-2.7920334	3.5616623
H	-1.1786124	-1.2093561	3.0890975
C	-3.2485252	-3.9116503	3.0900906
H	-3.5943472	-5.2100132	1.3972726
H	-2.7049803	-2.4463240	4.5859925
H	-3.9323059	-4.4505354	3.7479180
C	-0.2116022	-2.6077360	-1.2011318
C	0.5562176	-3.7813483	-1.1170168
C	-0.8417369	-2.2859172	-2.4101331
C	0.6774323	-4.6204920	-2.2242312
H	1.0645224	-4.0356032	-0.1856539
C	-0.7084957	-3.1218262	-3.5204940
H	-1.4314648	-1.3716810	-2.4738176
C	0.0491352	-4.2911921	-3.4292183
H	1.2698963	-5.5337925	-2.1463648
H	-1.1975780	-2.8572970	-4.4594541
H	0.1498923	-4.9475470	-4.2953411
C	1.0129616	3.5006810	-0.3278876
C	0.1031122	4.3768972	0.2873099
C	2.0850940	4.0344434	-1.0582658
C	0.2542515	5.7579452	0.1665919
H	-0.7181720	3.9679383	0.8818705
C	2.2290266	5.4180075	-1.1850893
H	2.8132237	3.3722349	-1.5286829
C	1.3154412	6.2815283	-0.5769354
H	-0.4554521	6.4270443	0.6559560
H	3.0652320	5.8219848	-1.7581868
H	1.4332530	7.3614928	-0.6770718
C	1.6709727	1.6356930	1.6367044
C	2.9978894	2.0764060	1.7595784
C	0.9586231	1.2527887	2.7801042
C	3.6071622	2.1084250	3.0121484
H	3.5563066	2.3885756	0.8757374
C	1.5722372	1.2884495	4.0340106
H	-0.0808702	0.9314439	2.6809185
C	2.8965369	1.7136375	4.1508484
H	4.6392444	2.4518108	3.1034081
H	1.0126614	0.9865791	4.9208203
H	3.3752860	1.7457538	5.1308070
O	3.4024769	-2.3879445	-1.7223810
O	4.6375109	-0.4367408	0.3324437
C	5.9478344	-0.4403094	0.8996130
H	6.5748669	0.1220171	0.1992550
H	5.9591386	0.0569171	1.8835081
H	6.3389761	-1.4656928	1.0001670
C	3.9520517	-3.1965395	-2.7627140
H	4.3557281	-4.0840451	-2.2633266
H	3.1751650	-3.5031789	-3.4816310
H	4.7645026	-2.6720713	-3.2911456
C	-5.9434471	-0.8790655	0.7955037
H	-5.0333120	-1.3638151	1.1624281
H	-6.6080141	-0.6662653	1.6434077
H	-6.4560113	-1.5393096	0.0854099

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TsIII_IVS.xyz
98
Energy = -2817.807631559
Rh  -1.2351188   0.3128552  -0.6568606
H   -2.1507865  -0.8230658  -1.3879826
H   -2.4017824   1.9202202   1.3671882
B   -2.6256790   0.7697040   1.0502347
H   -2.4136860  -0.0371509   1.9196302
C   -6.1072265   0.0523852  -0.2873775
C   -5.7274959   1.1248695  -1.0436957
H   -7.0272826  -0.5199586  -0.2829443
H   -6.2460220   1.6532237  -1.8351461
C   -4.0370372   0.6520567   0.3754255
N   -4.4670108   1.4831736  -0.6147340
N   -5.0589462  -0.2260193   0.5720178
C   -2.3662415   1.7406151  -1.8558032
C   -2.5208234   0.4322772  -2.4112092
H   -3.5179312  -0.0159510  -2.4565955
H   -1.8958710   0.1554247  -3.2655488
H   -1.6644139   2.4280784  -2.3342033
P   -0.2030715  -1.6083629   0.2028697
P    0.4078575   1.7863048   0.0110855
C    1.3907976  -1.4391815   1.1223683
C    2.4107138  -0.6553643   0.5455539
C    1.6067849  -2.0623631   2.3609200
C    3.6142848  -0.4619535   1.2623754
C    2.8074415  -1.8741577   3.0405471
H    0.8460171  -2.7073793   2.7946866
C    3.8077097  -1.0618157   2.5119705
H    2.9657791  -2.3640647   4.0026010
H    4.7314209  -0.9089822   3.0671221
C    1.5475361   1.0112881  -1.1992325
C    1.4444656   1.3973320  -2.5529446
C    2.3232038  -0.1090642  -0.8404266
C    2.1514947   0.7064289  -3.5309763
H    0.8148998   2.2408450  -2.8348588
C    3.0476094  -0.7861025  -1.8544511
C    2.9616484  -0.3766132  -3.1912134
H    2.0757888   1.0146498  -4.5749995
H    3.5077520  -0.9069893  -3.9692171
C   -3.5603250   2.4441986  -1.2370922
H   -3.2383055   3.1701601  -0.4780936
H   -4.1361569   2.9924803  -1.9994444
C   -1.2780184  -2.6566714   1.2608338
C   -1.9470268  -3.7578719   0.7031140
C   -1.5350882  -2.3197823   2.6019397
C   -2.8313466  -4.5173689   1.4723295
H   -1.7671851  -4.0346385  -0.3366240
C   -2.4081686  -3.0899214   3.3726428
H   -1.0446606  -1.4586304   3.0549046
C   -3.0587107  -4.1917317   2.8113331
H   -3.3318526  -5.3773467   1.0240356
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H   -2.5798037  -2.8244282   4.4172282
H   -3.7362267  -4.7959201   3.4167368
C    0.3195391  -2.7693933  -1.1326272
C    1.1175115  -3.8788011  -0.8043986
C   -0.0507533  -2.5707690  -2.4679064
C    1.5133185  -4.7791809  -1.7917166
H    1.4335760  -4.0357148   0.2283137
C    0.3555033  -3.4673506  -3.4595955
H   -0.6521420  -1.7029865  -2.7369968
C    1.1332790  -4.5758340  -3.1226284
H    2.1251652  -5.6417518  -1.5222692
H    0.0635366  -3.2961022  -4.4969642
H    1.4463162  -5.2808807  -3.8946281
C    0.3001754   3.5688318  -0.4106631
C   -0.7735996   4.2807365   0.1497593
C    1.2699708   4.2661235  -1.1476129
C   -0.8891543   5.6570092  -0.0437285
H   -1.5049931   3.7519927   0.7646108
C    1.1468973   5.6437217  -1.3442417
H    2.1278931   3.7394311  -1.5668746
C    0.0671108   6.3409981  -0.7991216
H   -1.7248073   6.1983755   0.4031144
H    1.9057569   6.1743179  -1.9217475
H   -0.0233354   7.4172750  -0.9530899
C    1.2057087   1.9090336   1.6529723
C    2.4042391   2.6231526   1.8110839
C    0.5602938   1.3752829   2.7750244
C    2.9612855   2.7744043   3.0792373
H    2.9048604   3.0561717   0.9436655
C    1.1205877   1.5340310   4.0439820
H   -0.3851154   0.8462800   2.6479301
C    2.3215723   2.2289618   4.1973574
H    3.8936579   3.3293261   3.1981748
H    0.6144089   1.1159943   4.9156286
H    2.7566965   2.3552474   5.1900409
O    3.7834659  -1.8461980  -1.4349067
O    4.5248155   0.3455163   0.6559542
C    5.7621779   0.5847865   1.3275158
H    6.3328343   1.2482213   0.6687170
H    5.5991862   1.0814673   2.2979831
H    6.3231316  -0.3513027   1.4805804
C    4.4981490  -2.6046945  -2.4117975
H    4.9986319  -3.4034836  -1.8540712
H    3.8115158  -3.0497968  -3.1495502
H    5.2531010  -1.9877211  -2.9253236
C   -5.0587046  -1.3092853   1.5477167
H   -5.2022147  -2.2700406   1.0371098
H   -4.0916197  -1.3168977   2.0576373
H   -5.8616861  -1.1567935   2.2805610
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TsIV_VS.xyz
98
Energy = -2817.815582085

Rh	1.7655691	0.2406750	-0.0137348
H	3.9358954	0.4387424	-0.9177908
H	0.8260313	2.9234350	0.4957440
B	1.7852744	2.2276732	0.7463889
H	2.6852044	2.3571810	-0.0796603
C	2.4152312	3.2277758	4.3350251
C	3.1809829	2.1007473	4.2684296
H	2.2397852	3.9188563	5.1510397
H	3.7876851	1.6103877	5.0203929
C	2.2272273	2.3850734	2.2489466
N	3.0533058	1.6017506	2.9890904
N	1.8362956	3.3870994	3.0935654
C	3.4555523	-0.1231894	1.1580638
C	4.4137136	0.4050145	0.0958525
H	4.7457622	1.4326473	0.2954334
H	5.2918720	-0.2475116	-0.0415407
H	3.5000884	-1.2234237	1.1811305
P	0.4310328	0.4864528	-1.9434214
P	0.1981247	-0.7341385	1.1831091
C	-1.3651778	0.7236674	-1.6561261
C	-2.0854100	-0.3181089	-1.0365059
C	-1.9814521	1.9561529	-1.9171790
C	-3.4385332	-0.0850123	-0.6841884
C	-3.3114717	2.1606841	-1.5589508
H	-1.4268901	2.7503858	-2.4145933
C	-4.0436950	1.1519226	-0.9370736
H	-3.7888609	3.1188149	-1.7710645
H	-5.0804561	1.3298305	-0.6574347
C	-0.6361463	-2.0619403	0.2036602
C	-0.3125774	-3.4146938	0.4020913
C	-1.5505317	-1.6974299	-0.8106217
C	-0.8581693	-4.3999323	-0.4145238
H	0.3371902	-3.7131843	1.2191323
C	-2.0854154	-2.7224347	-1.6337986
C	-1.7285982	-4.0625963	-1.4466095
H	-0.6021669	-5.4468037	-0.2443912
H	-2.1365469	-4.8415025	-2.0880616
C	3.6998812	0.3358968	2.5771061
H	3.3405789	-0.4236065	3.2843908
H	4.7797890	0.4712645	2.7666818
C	0.9515281	4.4908018	2.7335386
H	1.3267179	5.0027359	1.8407197
H	-0.0602534	4.1157954	2.5360285
H	0.9199147	5.1959185	3.5710414
C	0.9016542	-1.5210418	2.7001469
C	0.6195404	-0.9883088	3.9691757
C	1.8618994	-2.5469156	2.6075316
C	1.2602677	-1.4791838	5.1095129
H	-0.1029008	-0.1790927	4.0733083
C	2.4853112	-3.0503894	3.7488526
H	2.1491986	-2.9448880	1.6339490
C	2.1879855	-2.5168318	5.0064903
H	1.0240997	-1.0489092	6.0842589
H	3.2161287	-3.8549808	3.6529478
H	2.6804100	-2.9068973	5.8984343
C	-1.2525437	0.1679344	1.8689247
C	-2.2326164	-0.5920756	2.5318408
C	-1.4134962	1.5524581	1.7637820
C	-3.3394961	0.0353707	3.1011341
H	-2.1324527	-1.6768354	2.5989449
C	-2.5320305	2.1753280	2.3211640
H	-0.6754199	2.1320027	1.2125903
C	-3.4925431	1.4213968	2.9978040
H	-4.0903337	-0.5631229	3.6198082
H	-2.6621881	3.2536453	2.2104409
H	-4.3638071	1.9095354	3.4378169
C	0.5179177	-1.0021645	-3.0099643
C	-0.3772519	-1.1960038	-4.0737765
C	1.5191192	-1.9549691	-2.7740791
C	-0.2638446	-2.3230274	-4.8876224
H	-1.1696387	-0.4681852	-4.2567301
C	1.6249520	-3.0878135	-3.5817930
H	2.2159135	-1.8132801	-1.9422152
C	0.7333956	-3.2715826	-4.6412821
H	-0.9576771	-2.4618965	-5.7187432
H	2.4024448	-3.8273040	-3.3844003
H	0.8170925	-4.1540938	-5.2776616
C	0.9687838	1.8458637	-3.0599143
C	1.3803829	1.6069112	-4.3810952
C	1.0478108	3.1564026	-2.5539967
C	1.8401239	2.6561277	-5.1803885
H	1.3489351	0.5988249	-4.7933893
C	1.4951235	4.2022706	-3.3602024
H	0.7713440	3.3569121	-1.5193661
C	1.8929984	3.9562879	-4.6768640
H	2.1574915	2.4509289	-6.2040963
H	1.5420969	5.2139466	-2.9534227
H	2.2497413	4.7741931	-5.3047238
O	-4.0751538	-1.1275697	-0.0859542
O	-2.9443857	-2.3044115	-2.5999910
C	-5.4442805	-0.9621763	0.2786848
H	-5.7483784	-1.9154742	0.7247892
H	-5.5656707	-0.1557294	1.0206287
H	-6.0722585	-0.7523178	-0.6022719
C	-3.5380487	-3.2867780	-3.4481704
H	-4.1892869	-2.7309681	-4.1315422
H	-2.7735314	-3.8278785	-4.0293949
H	-4.1408088	-4.0051179	-2.8692421

TsV_VIS.xyz
98
Energy = -2817.803423396

Rh	-1.3315235	0.0072872	-0.3416420
H	-2.4698314	0.4752511	-2.8830948
H	-2.7917071	-0.4484706	1.7461913
B	-3.1133639	-0.3455246	0.5745626
H	-2.6329479	-1.2123186	-0.2965979
C	-6.9066486	-0.2982867	0.5916221
C	-6.5712770	0.9549257	0.1565659
H	-7.8758064	-0.7488122	0.7718441
H	-7.1911630	1.8059236	-0.0992630
C	-4.6748450	-0.2041655	0.4453037
N	-5.1949809	0.9789196	0.0732092
N	-5.7225170	-0.9970218	0.7715609
C	-3.0230722	1.3955588	-0.9835122
C	-3.3699393	0.8246120	-2.3567203
H	-4.0543622	-0.0352602	-2.2938653
H	-3.8538077	1.5882845	-2.9952277
H	-2.3296123	2.2335190	-1.0942571
P	0.2259500	-1.6561370	-0.1658071
P	0.2605492	1.6180654	-0.1259299
C	1.4765764	-1.4168035	1.1627905
C	2.4642336	-0.4276686	0.9871764
C	1.3718803	-2.0990357	2.3850018
C	3.3175156	-0.1205946	2.0756071
C	2.2259690	-1.7842984	3.4380787
H	0.6351617	-2.8889552	2.5137760
C	3.1895734	-0.7883816	3.2993294
H	2.1408336	-2.3225492	4.3834438
H	3.8426864	-0.5465545	4.1358473
C	1.9104669	1.2558657	-0.8755783
C	2.3066812	1.9012174	-2.0585892
C	2.7310048	0.2570867	-0.3130033
C	3.4911570	1.5444951	-2.6950525
H	1.7030716	2.7015899	-2.4790785
C	3.9267929	-0.0982341	-0.9879086
C	4.3003198	0.5371938	-2.1770123
H	3.7886100	2.0578095	-3.6107951
H	5.2171662	0.2585559	-2.6932173
C	-4.2446973	2.0278972	-0.3233465
H	-3.9701626	2.6106417	0.5689443
H	-4.7697118	2.6979454	-1.0257010
C	-5.6087970	-2.3804339	1.2197814
H	-6.1120860	-3.0502227	0.5106309
H	-4.5473136	-2.6480105	1.2704583
H	-6.0610044	-2.4915840	2.2137588
C	-0.2132593	3.2353256	-0.8777821
C	-0.3055722	4.4194091	-0.1334738
C	-0.5851119	3.2609355	-2.2362669
C	-0.7331118	5.6050451	-0.7390945
H	-0.0466805	4.4226056	0.9252674
C	-0.9984278	4.4466472	-2.8411382
H	-0.5651630	2.3374568	-2.8199117
C	-1.0720394	5.6251408	-2.0922621
H	-0.7971654	6.5180996	-0.1448702
H	-1.2724587	4.4480767	-3.8974083
H	-1.4000429	6.5534911	-2.5623791
C	0.6519305	2.0354978	1.6146638
C	1.7540934	2.8525498	1.9158819
C	-0.1619013	1.5605045	2.6511932
C	2.0280372	3.1936181	3.2400495
H	2.4059958	3.2082125	1.1161985
C	0.1239814	1.8939645	3.9760010
H	-1.0068047	0.9135404	2.4051027
C	1.2166377	2.7122247	4.2719498
H	2.8822800	3.8339453	3.4671287
H	-0.5067109	1.5105913	4.7797523
H	1.4379403	2.9751679	5.3077842
C	1.2032200	-2.0709394	-1.6558900
C	2.3007393	-2.9439181	-1.5817879
C	0.8278226	-1.5335541	-2.8944906
C	3.0067128	-3.2753426	-2.7378749
H	2.6093874	-3.3516092	-0.6175462
C	1.5437851	-1.8588164	-4.0475487
H	-0.0237922	-0.8494590	-2.9398310
C	2.6320487	-2.7311599	-3.9704741
H	3.8545718	-3.9600031	-2.6763683
H	1.2527117	-1.4295131	-5.0074670
H	3.1899249	-2.9883990	-4.8724110
C	-0.6307712	-3.2379038	0.2523486
C	-0.5247252	-4.3754756	-0.5597350
C	-1.4681518	-3.2908410	1.3818380
C	-1.2322554	-5.5403922	-0.2459806
H	0.1055473	-4.3580842	-1.4485825
C	-2.1559374	-4.4597749	1.7036278
H	-1.5899609	-2.4058295	2.0080412
C	-2.0427856	-5.5903870	0.8873832
H	-1.1420869	-6.4130939	-0.8947685
H	-2.7795945	-4.4907035	2.5996202
H	-2.5843474	-6.5044007	1.1361329
O	4.2358126	0.8547576	1.8410806
O	4.6498194	-1.0934708	-0.4080214
C	5.1383947	1.1967729	2.8918654
H	5.7814433	1.9845067	2.4842355
H	4.5992481	1.5827307	3.7726472
H	5.7573026	0.3336924	3.1864056
C	5.8727937	-1.4874841	-1.0286852
H	6.2806512	-2.2845733	-0.3974810
H	5.6982340	-1.8774838	-2.0449934
H	6.5889277	-0.6508921	-1.0719853

VIR.1.xyz
121
Energy = -3226.384437318
Rh -0.0462269 -0.7169601   0.4994739
H   -1.8140848 -0.4418499   0.3962287
H   -1.8330185 -2.8911093   3.1705779
B   -1.9714415 -1.7449099   0.5390724
H   -0.8160567 -2.2638298   0.9214952
C   -3.3663748 -3.2027219 -2.6935440
C   -4.3505158 -3.3390270 -1.7471950
H   -3.3609754 -3.4612771 -3.7462325
H   -5.3631741 -3.7135777 -1.8313174
C   -2.5626587 -2.4114832 -0.7678861
N   -3.8200430 -2.8594365 -0.5763557
N   -2.2709471 -2.6287012 -2.0712587
C   -3.1565551 -2.1251150   1.6078643
C   -2.6994833 -3.2238824   2.5820411
H   -2.3912964 -4.1328344   2.0405263
H   -3.4998811 -3.5072572   3.2832098
H   -3.4502280 -1.2404563   2.1930513
P   2.0054895 -1.4689394   0.9421904
P   0.7295287   1.2066102 -0.3104108
C   3.4144600 -0.3106556   1.1605881
C   3.8231594   0.5348034   0.1087530
C   4.0108817 -0.2043432   2.4279017
C   4.8282961   1.4988513   0.3731618
C   5.0095165   0.7370028   2.6556222
H   3.6937744 -0.8595309   3.2370365
C   5.4195268   1.5950232   1.6381935
H   5.4713935   0.8098403   3.6414260
H   6.1901154   2.3380953   1.8361191
C   1.9745344   0.8792833 -1.6291347
C   1.5659904   0.8800338 -2.9728055
C   3.2790445   0.4698131 -1.2817556
C   2.4396451   0.4589566 -3.9706843
H   0.5665932   1.2204924 -3.2398581
C   4.1477898   0.0419848 -2.3171403
C   3.7258722   0.0276850 -3.6522396
H   2.1182962   0.4689982 -5.0136408
H   4.3960580 -0.3030626 -4.4436914
C   -4.3710910 -2.5852485   0.7605616
H   -4.8552170 -3.4944330   1.1470768
H   -5.1305707 -1.7991230   0.6392896
C   -1.0051345 -2.2874099 -2.7120208
H   -0.3729274 -1.7738468 -1.9679103
H   -0.4934494 -3.1945453 -3.0584277
H   -1.1864225 -1.6197270 -3.5640770
O   5.1368302   2.3227165 -0.6652651
O   5.3890964 -0.3496758 -1.9180554
C   6.1579157   3.3000166 -0.4702027
H   6.2430715   3.8324691 -1.4238045
H   5.8855172   4.0133744   0.3252133

H   7.1235935   2.8287696 -0.2253050
C   6.3171202 -0.7745598 -2.9151089
H   7.2353960 -1.0280846 -2.3740331
H   5.9505090 -1.6646087 -3.4529345
H   6.5281540   0.0308696 -3.6370479
C   -0.6156648   2.1584434 -1.1485931
C   -0.7460966   3.5515362 -1.0328933
C   -1.5743669   1.4552227 -1.8975341
C   -1.8019581   4.2182798 -1.6610737
H   -0.0326162   4.1244562 -0.4415206
C   -2.6208883   2.1209941 -2.5343413
H   -1.5186469   0.3679929 -1.9530311
C   -2.7370668   3.5080980 -2.4166251
H   -1.8916570   5.3006498 -1.5532639
H   -3.3691997   1.5468675 -3.0817121
H   -3.5643435   4.0310495 -2.8992314
C   1.4840533   2.4567013   0.7942932
C   2.2642288   3.5094795   0.2897074
C   1.2182703   2.3903445   2.1684692
C   2.7617556   4.4859696   1.1525671
H   2.4975110   3.5533383 -0.7758184
C   1.7228546   3.3662923   3.0299800
H   0.6219553   1.5587069   2.5526133
C   2.4915643   4.4165644   2.5227202
H   3.3649252   5.3037277   0.7536624
H   1.5199227   3.3033202   4.1003509
H   2.8853150   5.1799617   3.1958398
C   1.9185847 -2.3719121   2.5420804
C   2.6738393 -3.5268676   2.7927191
C   1.0627367 -1.8793312   3.5407178
C   2.5736351 -4.1757079   4.0254746
H   3.3393330 -3.9237043   2.0246336
C   0.9692049 -2.5267331   4.7727436
H   0.4612457 -0.9898187   3.3327607
C   1.7241174 -3.6777484   5.0163037
H   3.1617672 -5.0760598   4.2107655
H   0.3008575 -2.1360914   5.5420213
H   1.6472089 -4.1889170   5.9773583
C   2.6119603 -2.7534503 -0.2213769
C   3.9653111 -2.8659851 -0.5677719
C   1.6954483 -3.6921117 -0.7223809
C   4.3894386 -3.8903431 -1.4183081
H   4.6896621 -2.1483578 -0.1830226
C   2.1236014 -4.7184076 -1.5627746
H   0.6433220 -3.6175193 -0.4406275
C   3.4725081 -4.8158773 -1.9191711
H   5.4457224 -3.9677465 -1.6825465
H   1.4044780 -5.4488531 -1.9385244
H   3.8073532 -5.6170022 -2.5800040
C   -3.7094724   1.7839404   2.2836568
C   -2.7558020   2.3195092   3.0499011
H   -2.7450069   2.1777396   4.1311241

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H   -1.9442918   2.9107893   2.6174562        C    1.3966077   1.2339257  -1.7863132
C   -3.7258849   1.8914652   0.7896918        C    0.8010252   1.5724579  -3.0121526
H   -2.9734905   2.6133654   0.4400355        C    2.6057086   0.5086966  -1.7553808
H   -3.4947656   0.9230249   0.3241897        C    1.3905339   1.1756037  -4.2089164
H   -4.5158595   1.1954282   2.7346751        H   -0.1229532   2.1488223  -3.0299343
N   -5.0362451   2.2746049   0.2599073        C    3.1848510   0.1164909  -2.9880973
C   -5.7046058   3.4351128   0.6164629        C    2.5731090   0.4376413  -4.2068689
C   -6.8605109   3.4561555  -0.1032533        H    0.9277003   1.4473743  -5.1593191
H   -5.3053568   4.1281041   1.3470967        H    3.0236218   0.1359862  -5.1508799
N   -6.8658352   2.3118684  -0.8821723        C   -4.2884036  -3.3983455  -0.3096095
H   -7.6701926   4.1756947  -0.1251253        H   -4.4370064  -4.4319953   0.0377726
C   -7.9296626   1.9122904  -1.7918031        H   -5.2642363  -2.9964642  -0.6219898
H   -7.5008133   1.6647185  -2.7706319        C   -0.6488816  -1.7397658  -3.0534316
H   -8.4440425   1.0222135  -1.4056504        H   -0.3873858  -1.0836856  -2.2097248
H   -8.6422892   2.7383454  -1.8913851        H    0.2120726  -2.3751508  -3.2954090
C   -5.7430716   1.5695043  -0.6690429        H   -0.9234573  -1.1331632  -3.9257830
B   -5.4107307   0.1921065  -1.3879965        O    4.8861088   1.8317878  -1.3096875
H   -5.5089834   0.3531892  -2.6015375        O    4.3535293  -0.5781320  -2.8967216
H   -4.2862608  -0.1884441  -1.1027814        C    6.1097995   2.5576908  -1.2073376
H   -6.2574095  -0.6336437  -1.0457843        H    6.1520047   3.1928282  -2.0990476
                                              H    6.1271590   3.1911639  -0.3050689
VIIa.xyz                                      H    6.9797295   1.8808992  -1.1976141
121                                           C    5.0071054  -0.9691381  -4.1033439
Energy = -3226.385457261                      H    5.9166112  -1.4932079  -3.7897650
Rh  -0.5471846  -0.2901995   0.4323020        H    4.3788338  -1.6513280  -4.6999557
H   -2.5748806  -0.4639735  -0.2862489        H    5.2806477  -0.0932855  -4.7136689
H   -2.5271169  -2.6685112   2.6319178        C   -0.7645452   2.8391905  -0.6678572
B   -2.3974891  -1.6755610  -0.0856592        C   -0.5545369   4.2152370  -0.4919992
H   -1.3247862  -1.8758646   0.6304731        C   -1.9947593   2.4096206  -1.1946363
C   -2.3959022  -3.5250507  -3.4311352        C   -1.5458527   5.1353232  -0.8431649
C   -3.4273050  -4.0539552  -2.6995782        H    0.3842943   4.5780536  -0.0735642
H   -2.0482354  -3.7571425  -4.4312773        C   -2.9836889   3.3284048  -1.5452143
H   -4.1528946  -4.8185422  -2.9504896        H   -2.1745316   1.3400255  -1.3253555
C   -2.3984978  -2.4985031  -1.4429137        C   -2.7612120   4.6964713  -1.3712478
N   -3.4007228  -3.4047079  -1.4856271        H   -1.3617682   6.2023328  -0.7043768
N   -1.7811777  -2.5640820  -2.6455929        H   -3.9339605   2.9735914  -1.9482700
C   -3.5820555  -2.4948505   0.7340228        H   -3.5342506   5.4171782  -1.6429307
C   -3.0198848  -3.3223707   1.8991620        C    1.6639802   2.4762761   0.8497434
H   -2.2628577  -4.0439035   1.5494561        C    2.5455623   3.4362235   0.3262130
H   -3.8048818  -3.8915115   2.4225615        C    1.6435255   2.2364564   2.2307838
H   -4.3312636  -1.7996569   1.1378308        C    3.3812198   4.1566942   1.1795646
P    1.3027403  -1.4859152   0.5078618        H    2.5945769   3.6017584  -0.7517922
P    0.4915339   1.5565791  -0.2164653        C    2.4858856   2.9561734   3.0807871
C    2.9444313  -0.6412086   0.5307865        H    0.9671814   1.4768626   2.6293922
C    3.3588963   0.2399970  -0.4924185        C    3.3512190   3.9194983   2.5574684
C    3.7506362  -0.8174914   1.6689964        H    4.0629466   4.9029308   0.7671177
C    4.5796522   0.9444270  -0.3225430        H    2.4717004   2.7559132   4.1534150
C    4.9551988  -0.1351005   1.7978202        H    4.0099738   4.4810480   3.2220436
H    3.4309970  -1.4878417   2.4637213        C    1.2354064  -2.3880944   2.1176945
C    5.3760593   0.7514071   0.8105951        C    1.8580458  -3.6337616   2.2989977
H    5.5708076  -0.2864059   2.6858575        C    0.5372745  -1.8092835   3.1894722
H    6.3106406   1.2956905   0.9332375        C    1.7796995  -4.2865273   3.5304686
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H	2.4057709	-4.0969113	1.4769894	H	-0.4407462	-4.6682799	-3.8333076
C	0.4606176	-2.4649834	4.4189481	H	-2.3382908	-6.1324043	-2.4186936
H	0.0346744	-0.8490708	3.0468022	C	-1.6761873	-3.1554333	-1.2201020
C	1.0799189	-3.7052028	4.5914044	N	-2.3220653	-4.3419023	-1.1894590
H	2.2661829	-5.2548247	3.6598725	N	-0.8727397	-3.1935871	-2.3073760
H	-0.0928684	-2.0059220	5.2397910	C	-3.1329444	-3.2306800	0.7835171
H	1.0151704	-4.2214558	5.5507118	C	-2.4947110	-3.6619228	2.1105487
C	1.5162192	-2.8828814	-0.6748591	H	-1.5080084	-4.1280919	1.9529410
C	2.5997974	-2.9727713	-1.5588010	H	-3.1186309	-4.3869734	2.6578939
C	0.5294882	-3.8851525	-0.7064365	H	-4.1163662	-2.7888530	1.0055698
C	2.6723916	-4.0195565	-2.4831725	P	1.3659863	-1.1442355	0.9469299
H	3.3995516	-2.2346023	-1.5256378	P	0.2471466	1.6393477	-0.3724129
C	0.6123025	-4.9361989	-1.6171414	C	2.8256933	-0.0197416	1.0877205
H	-0.3052373	-3.8444036	-0.0048175	C	3.2666628	0.7780723	0.0094440
C	1.6781294	-4.9988539	-2.5225929	C	3.4367921	0.1098244	2.3468838
H	3.5231283	-4.0755980	-3.1651992	C	4.3110699	1.7109740	0.2410773
H	-0.1581682	-5.7094670	-1.6221861	C	4.4720670	1.0174907	2.5424235
H	1.7411426	-5.8186263	-3.2400487	H	3.0962218	-0.4977096	3.1825123
C	-5.4647842	0.7001753	0.1432440	C	4.9126858	1.8259177	1.4983439
C	-6.6521042	0.6015854	-0.4589552	H	4.9367801	1.1050289	3.5257430
H	-6.7353442	0.3848047	-1.5248082	H	5.7110444	2.5456793	1.6696204
H	-7.5875754	0.7248500	0.0929048	C	1.4361286	1.2091809	-1.7158469
C	-5.2870380	0.9554752	1.6117747	C	1.0229996	1.2466103	-3.0575746
H	-6.2595039	1.0840925	2.1094935	C	2.7158948	0.7218881	-1.3789393
H	-4.7581292	0.1200797	2.0921337	C	1.8662728	0.7851641	-4.0639773
H	-4.5380372	0.5654235	-0.4226031	H	0.0425188	1.6428047	-3.3170261
N	-4.4712011	2.1440275	1.8771484	C	3.5578570	0.2635200	-2.4232281
C	-4.9148799	3.4411970	1.6884912	C	3.1291205	0.2818892	-3.7564137
C	-3.8886781	4.2602227	2.0493960	H	1.5412183	0.8233217	-5.1052283
H	-5.9061993	3.6642304	1.3133504	H	3.7800134	-0.0707234	-4.5545732
N	-2.8445032	3.4455798	2.4440405	C	-3.3622040	-4.4474208	-0.1509034
H	-3.8118097	5.3405366	2.0534165	H	-3.2681637	-5.4173513	0.3611403
C	-1.5568916	3.9164653	2.9346165	H	-4.3433400	-4.4149274	-0.6486868
H	-1.4071187	3.5906625	3.9714828	C	0.0087900	-2.1114107	-2.7261784
H	-0.7467162	3.5111674	2.3186029	H	-0.0382177	-1.3220356	-1.9602607
H	-1.5394653	5.0102051	2.8807677	H	1.0417703	-2.4730323	-2.8028438
C	-3.1872336	2.1299167	2.3387035	H	-0.3178870	-1.7096329	-3.6940572
B	-2.2568883	0.8928855	2.6610690	O	4.6469746	2.4902598	-0.8241104
H	-2.8726036	-0.1414830	2.7973917	O	4.7868531	-0.1822309	-2.0381336
H	-1.4699153	0.8071658	1.6482249	C	5.6999467	3.4380475	-0.6593133
H	-1.5138695	1.1361619	3.5953292	H	5.8014665	3.9385583	-1.6286342
				H	5.4512362	4.1836494	0.1139696
VIIb.xyz				H	6.6502175	2.9429578	-0.4008228
121				C	5.6939982	-0.6264256	-3.0458818
Energy = -3226.386176385				H	6.6050738	-0.9210314	-2.5135916
Rh	-0.6138174	-0.2173161	0.4725071	H	5.2936457	-1.4951225	-3.5948612
H	-2.7859257	-1.2378910	-0.5976845	H	5.9301348	0.1810906	-3.7576360
H	-2.3319131	-2.7927803	2.7629560	C	-1.0741327	2.6022261	-1.2452520
B	-2.1903198	-2.1678851	-0.0866646	C	-1.1369003	4.0026619	-1.2522110
H	-1.2573701	-1.8547267	0.7587908	C	-2.0845605	1.8817944	-1.9081661
C	-1.0143019	-4.4141048	-2.9494636	C	-2.1809954	4.6655633	-1.9046030
C	-1.9397820	-5.1395553	-2.2471239	H	-0.3747114	4.5878512	-0.7377955

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C   -3.1201961    2.5438794   -2.5665186
H   -2.0587533    0.7888814   -1.8881100
C   -3.1742006    3.9406229   -2.5640037
H   -2.2116371    5.7568991   -1.8985149
H   -3.8936717    1.9685238   -3.0785185
H   -3.9874698    4.4594846   -3.0739897
C    1.1139395    2.9193893    0.6170683
C    1.8781267    3.9315893    0.0129328
C    0.9801861    2.8966062    2.0120228
C    2.4792117    4.9168917    0.7964189
H    2.0209379    3.9348289   -1.0693650
C    1.5892486    3.8803378    2.7939122
H    0.4083751    2.0899505    2.4759581
C    2.3341953    4.8941763    2.1871724
H    3.0677798    5.7032404    0.3199497
H    1.4893556    3.8483246    3.8801283
H    2.8105942    5.6627874    2.7981268
C    1.1633210   -1.8154262    2.6556432
C    1.9082883   -2.9080842    3.1266762
C    0.2311155   -1.2051875    3.5097963
C    1.7162860   -3.3834122    4.4253256
H    2.6414489   -3.3912611    2.4794813
C    0.0422632   -1.6818206    4.8074763
H   -0.3594786   -0.3622611    3.1395088
C    0.7823471   -2.7738153    5.2670631
H    2.2996468   -4.2349654    4.7797251
H   -0.6918919   -1.2020567    5.4569626
H    0.6311750   -3.1514704    6.2797054
C    2.0092719   -2.6256079    0.0600398
C    3.2418132   -2.6412822   -0.6053228
C    1.2208647   -3.7895033    0.0563912
C    3.6572012   -3.7844793   -1.2951027
H    3.8924872   -1.7686795   -0.5791301
C    1.6443763   -4.9336977   -0.6169685
H    0.2750609   -3.8013569    0.5996655
C    2.8599057   -4.9301794   -1.3098511
H    4.6212396   -3.7817765   -1.8076726
H    1.0241525   -5.8315321   -0.6002732
H    3.1911637   -5.8240989   -1.8409087
C   -5.5498006   -0.1579270   -1.0115184
C   -6.6825304   -0.5737358   -1.5821718
H   -6.7323228   -0.8144560   -2.6446820
H   -7.6013335   -0.7013384   -1.0039747
C   -5.4122730    0.1398721    0.4516476
H   -6.3662208   -0.0195598    0.9763145
H   -4.6504360   -0.5065526    0.9094359
H   -4.6360909   -0.0452536   -1.6018257
N   -4.9716952    1.5193467    0.7016287
C   -5.7167267    2.6394812    0.3859162
C   -4.9780257    3.7188148    0.7658475
H   -6.6881510    2.5717988   -0.0887348
N   -3.7976689    3.2314659    1.2977738
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H   -5.1860079    4.7798595    0.6996723
C   -2.7534314    4.0789114    1.8624026
H   -3.0120470    4.3662512    2.8907086
H   -1.8073451    3.5320077    1.8679837
H   -2.6490226    4.9759875    1.2417855
C   -3.7819924    1.8706495    1.2656263
B   -2.6219477    0.8850127    1.7291783
H   -3.0787073   -0.1282302    2.2150649
H   -2.1747235    0.6189234    0.5385933
H   -1.8286280    1.4482564    2.4489320
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VIIc.xyz
121
Energy = -3226.392656199
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Rh  -0.8214754   -0.0861804    0.1105257
P    0.4345750   -1.7062166    0.9957764
P    0.9712681    0.8842083   -0.7923327
C    0.4402102    1.8347910   -2.2896939
C    0.9501794    3.0894338   -2.6512070
C   -0.5269810    1.2355690   -3.1186450
C    0.5238798    3.7175446   -3.8264084
H    1.6842555    3.5866732   -2.0171808
C   -0.9490736    1.8614132   -4.2921616
H   -0.9422223    0.2654732   -2.8320167
C   -0.4193861    3.1040929   -4.6536232
H    0.9388944    4.6904033   -4.0970751
H   -1.6888207    1.3738836   -4.9298116
H   -0.7424651    3.5921633   -5.5746949
C    2.2184509   -0.2892369   -1.4884909
C    3.0562812   -1.0000225   -0.6063358
C    2.2654109   -0.5503598   -2.8669151
C    3.9276806   -1.9821920   -1.1378718
C    3.1346486   -1.5155358   -3.3672765
H    1.6300574    0.0036316   -3.5551452
C    3.9638433   -2.2392595   -2.5133985
H    3.1673579   -1.7101348   -4.4405450
H    4.6297226   -2.9981129   -2.9201175
C    2.0350191    2.0583903    0.1430869
C    3.2388935    2.5549652   -0.3837977
C    1.6480850    2.4308900    1.4357759
C    4.0167606    3.4431988    0.3595114
H    3.5827894    2.2237729   -1.3654244
C    2.4384937    3.3016470    2.1867365
H    0.7415335    1.9848874    1.8495370
C    3.6178708    3.8192937    1.6457080
H    4.9476623    3.8291159   -0.0599557
H    2.1507636    3.5591884    3.2081107
H    4.2360756    4.5017779    2.2316311
C    0.9556910   -3.1736326    0.0236339
C    1.9097518   -4.0783206    0.5190827
C    0.3831623   -3.3967430   -1.2349189
C    2.2631994   -5.2017285   -0.2283869
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H	2.3925295	-3.8920218	1.4801879
C	0.7484552	-4.5152432	-1.9855750
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C	1.6835627	-5.4221073	-1.4816711
H	2.9995671	-5.9041845	0.1665451
H	0.3042568	-4.6764467	-2.9693806
H	1.9659342	-6.2988673	-2.0671281
C	-0.4621104	-2.4186545	2.4488366
C	-1.1940146	-1.5366027	3.2630474
C	-0.4874631	-3.7882220	2.7478555
C	-1.9205532	-2.0097434	4.3553965
H	-1.2038573	-0.4721372	3.0184730
C	-1.2261179	-4.2629115	3.8353951
H	0.0532906	-4.4969861	2.1208550
C	-1.9412786	-3.3775998	4.6435311
H	-2.4797023	-1.3090228	4.9782288
H	-1.2418278	-5.3333174	4.0476157
H	-2.5159425	-3.7515203	5.4925520
C	2.0196591	-1.0988791	1.7204017
C	2.1265366	-0.8787124	3.1028784
C	3.0848239	-0.7540071	0.8645796
C	3.2844453	-0.3168615	3.6336267
H	1.3104548	-1.1593717	3.7667689
C	4.2484637	-0.1736777	1.4264428
C	4.3462882	0.0435859	2.8060429
H	3.3651031	-0.1581895	4.7104410
H	5.2411803	0.4890664	3.2368460
O	5.2215510	0.1638189	0.5376691
O	4.6830663	-2.6501884	-0.2251282
C	6.4251414	0.7359176	1.0438254
H	7.0588267	0.9150023	0.1681484
H	6.2293522	1.6926814	1.5560088
H	6.9393876	0.0465786	1.7333015
C	5.5811114	-3.6513371	-0.6995988
H	6.0775896	-4.0498219	0.1920966
H	5.0397288	-4.4638844	-1.2115950
H	6.3362449	-3.2243460	-1.3796851
C	-0.9966441	5.3598252	1.4122455
C	-1.3065980	5.4724458	0.0915015
C	-1.7794689	3.3543723	0.7255213
N	-1.2965438	4.0605708	1.7854629
H	-0.5876393	6.0806695	2.1098354
H	-1.2339597	6.3123262	-0.5887890
N	-1.7846105	4.2386289	-0.3087790
C	-2.3377450	3.9593919	-1.6364221
H	-2.3808513	2.8658098	-1.7259844
H	-1.6309732	4.3199353	-2.3950600
C	-3.6951470	4.5731695	-1.8186227
H	-4.4216825	4.3702349	-1.0244684
C	-4.0381268	5.3077791	-2.8787916
H	-3.3230025	5.5251698	-3.6762585
H	-5.0445781	5.7110816	-2.9941220

C	-1.1831013	3.5704874	3.1524699
B	-2.2818507	1.8452809	0.6938068
H	-3.4921947	1.8139213	0.5495281
H	-1.8539737	1.3188487	-0.4110670
H	-1.9672894	1.2524816	1.7104743
H	-2.0178785	3.9466849	3.7594668
H	-1.2151615	2.4772934	3.1394221
H	-0.2349100	3.9122867	3.5838749
H	-2.2674343	-0.9773307	0.6495393
B	-2.7736351	-1.5657896	-0.4049859
H	-2.1905448	-1.3680234	-1.4599543
C	-4.2957296	-1.0948509	-0.3497014
C	-3.0277826	-3.1306682	0.0600736
N	-5.0325000	-1.9197630	0.4275439
N	-5.1580851	-0.1753195	-0.8396002
C	-3.3174888	-4.0449895	-1.1372225
H	-2.1859362	-3.5437734	0.6318127
C	-4.2576003	-3.0428225	0.9921554
C	-6.3509630	-1.5260717	0.4572442
C	-6.4338283	-0.4206612	-0.3477818
C	-4.8077993	0.8614222	-1.7981185
H	-2.4437484	-4.1025664	-1.8004658
H	-4.1585060	-3.6662686	-1.7412088
H	-3.5675824	-5.0716591	-0.8231089
H	-4.8866884	-3.9457275	1.0026722
H	-3.9729446	-2.7950732	2.0268366
H	-7.1169445	-2.0492998	1.0171009
H	-7.2857670	0.1907485	-0.6221038
H	-3.7467794	0.7509572	-2.0440285
H	-5.4104192	0.7482869	-2.7090688
H	-4.9741713	1.8554720	-1.3651078

TsVII_IR.xyz
121
Energy = -3226.365402536

Rh	-0.3119041	0.1507853	1.3354825
P	1.2119957	-1.4107415	1.3417581
P	1.0129356	1.5038536	0.1764392
C	-0.0611568	2.8757554	-0.4240811
C	0.2468714	4.2278380	-0.2044708
C	-1.2895312	2.5468376	-1.0276010
C	-0.6477902	5.2290125	-0.5905350
H	1.1851636	4.5061121	0.2754251
C	-2.1728105	3.5511524	-1.4228030
H	-1.5557449	1.4991054	-1.1896925
C	-1.8567780	4.8949238	-1.2035679
H	-0.3943194	6.2750655	-0.4099945
H	-3.1169960	3.2831607	-1.9009652
H	-2.5536393	5.6792005	-1.5046934
C	1.7249778	0.6788935	-1.3024691
C	2.7946402	-0.2219182	-1.1191891
C	1.1126136	0.8103145	-2.5565266

C	3.2139414	-1.0042026	-2.2226619
C	1.5485282	0.0356872	-3.6268353
H	0.2866220	1.5050291	-2.6929636
C	2.5880352	-0.8776123	-3.4690672
H	1.0623573	0.1294217	-4.5989912
H	2.9027814	-1.4891591	-4.3126591
C	2.4512093	2.3638805	0.9229955
C	3.3311641	3.1001297	0.1123061
C	2.6738051	2.3075866	2.3041416
C	4.4032836	3.7843077	0.6844940
H	3.1842460	3.1240987	-0.9691556
C	3.7542675	2.9825135	2.8734961
H	2.0112105	1.6985494	2.9219492
C	4.6165772	3.7269388	2.0653031
H	5.0789795	4.3594507	0.0488291
H	3.9284088	2.9200486	3.9488315
H	5.4596429	4.2581967	2.5101695
C	1.0566491	-2.6058154	-0.0381892
C	2.0388431	-3.5901108	-0.2420928
C	-0.0391944	-2.5264283	-0.9078424
C	1.9077711	-4.4944350	-1.2959094
H	2.9135019	-3.6370570	0.4095823
C	-0.1533302	-3.4187289	-1.9745659
H	-0.7820800	-1.7387367	-0.7700659
C	0.8150813	-4.4070299	-2.1651584
H	2.6690354	-5.2623199	-1.4461725
H	-0.9928925	-3.3179683	-2.6641022
H	0.7249193	-5.1074566	-2.9976414
C	0.9791038	-2.3875382	2.8837371
C	0.9137707	-1.6910548	4.1043686
C	0.7866384	-3.7751779	2.8815975
C	0.6839062	-2.3711882	5.2987323
H	1.0388120	-0.6052493	4.1052742
C	0.5419624	-4.4533069	4.0797392
H	0.8168078	-4.3300046	1.9435378
C	0.4940877	-3.7573217	5.2881348
H	0.6490384	-1.8201410	6.2403789
H	0.3896255	-5.5338094	4.0641534
H	0.3066101	-4.2913332	6.2210802
C	2.9967142	-0.9739302	1.3203565
C	3.7821435	-1.1387707	2.4724969
C	3.5399082	-0.3723649	0.1668257
C	5.1025451	-0.6988744	2.4853259
H	3.3665895	-1.6221720	3.3548682
C	4.8790490	0.0880546	0.2137576
C	5.6544877	-0.0753282	1.3684047
H	5.7122804	-0.8383733	3.3794876
H	6.6833719	0.2785803	1.4006460
O	5.3247321	0.7046122	-0.9129977
O	4.2280947	-1.8747206	-1.9714924
C	6.6644281	1.1940521	-0.9275829
H	6.8042912	1.6428781	-1.9171118

H	6.8178571	1.9619746	-0.1512618
H	7.3924735	0.3781473	-0.7892994
C	4.6708087	-2.7167220	-3.0341862
H	5.4727183	-3.3308757	-2.6098043
H	3.8574201	-3.3704452	-3.3896784
H	5.0682019	-2.1271283	-3.8765905
C	-5.5790039	-0.6785322	3.6879330
C	-4.7817369	0.1186810	4.4551709
C	-3.5987403	-0.4708080	2.6254307
N	-4.8397401	-1.0312831	2.5758758
H	-6.5945423	-1.0228294	3.8421946
H	-4.9688371	0.6041262	5.4055657
N	-3.5748796	0.2317095	3.7933277
C	-2.4362241	1.0212742	4.2808101
H	-1.5413504	0.3806820	4.2759773
H	-2.6680469	1.2740223	5.3270994
C	-2.1987926	2.2611820	3.4665895
H	-3.0885372	2.8211620	3.1627840
C	-0.9771315	2.6874630	3.1337426
H	-0.0835172	2.1368853	3.4346915
H	-0.8261157	3.6048395	2.5648468
C	-5.3215927	-1.9068802	1.5095263
B	-2.4681569	-0.6265706	1.5287700
H	-2.7712582	-1.4727861	0.7232888
H	-2.2608691	0.4782445	0.9592457
H	-1.4147512	-1.0098135	2.1820983
H	-4.7044143	-2.8111253	1.4549120
H	-6.3586214	-2.1809605	1.7306358
H	-5.2739082	-1.3926360	0.5433698
H	-1.7182201	-0.2990733	-2.2581119
B	-2.5833544	-0.6446012	-3.0582924
H	-2.0790999	-1.3569710	-3.9147549
C	-3.2721883	0.6674347	-3.6365502
C	-3.9359320	-1.2763181	-2.3153667
N	-4.4702890	0.9217928	-3.0622928
N	-3.0650279	1.6804722	-4.5118433
C	-4.6716898	-2.2892987	-3.1995304
H	-3.6730264	-1.7532778	-1.3580789
C	-4.8339329	-0.0535147	-2.0182581
C	-5.0244001	2.0868026	-3.5523690
C	-4.1348339	2.5681511	-4.4754946
C	-1.8648370	1.8190927	-5.3220594
H	-4.0286868	-3.1557246	-3.4089132
H	-4.9368536	-1.8491279	-4.1749721
H	-5.6033132	-2.6628126	-2.7388895
H	-5.9164935	-0.2552253	-2.0709786
H	-4.6046493	0.3988221	-1.0379465
H	-5.9881497	2.4691655	-3.2377436
H	-4.1821900	3.4444540	-5.1119765
H	-1.3374480	0.8588471	-5.3064177
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H	-1.2117062	2.6019587	-4.9110621

TsVII_IS.xyz
121
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P	1.2981257	1.2568772	-1.1225195
C	0.5651498	1.8818276	-2.6881899
C	1.0462321	3.0171400	-3.3594491
C	-0.5905925	1.2389624	-3.1706911
C	0.3891904	3.4935840	-4.4958840
H	1.9322242	3.5380339	-2.9960574
C	-1.2300193	1.7092038	-4.3182062
H	-0.9935397	0.3584827	-2.6618774
C	-0.7463296	2.8400870	-4.9811212
H	0.7736630	4.3773796	-5.0078934
H	-2.1005327	1.1701754	-4.6970453
H	-1.2487428	3.2091357	-5.8768997
C	2.1197864	-0.3349098	-1.5339205
C	3.0056038	-0.9022603	-0.5955165
C	1.7667210	-1.0387847	-2.6945043
C	3.5217355	-2.1961870	-0.8477748
C	2.2880577	-2.3094847	-2.9203473
H	1.0845725	-0.6012225	-3.4206730
C	3.1591142	-2.8966335	-2.0047103
H	2.0081659	-2.8549504	-3.8228086
H	3.5487120	-3.8952434	-2.1941340
C	2.6914928	2.3991444	-0.7795857
C	3.8104440	2.4446244	-1.6272609
C	2.6335496	3.2517770	0.3308863
C	4.8426417	3.3479585	-1.3743790
H	3.8786875	1.7624371	-2.4767943
C	3.6725320	4.1472984	0.5878273
H	1.7795563	3.1789332	1.0086075
C	4.7751788	4.2006030	-0.2679783
H	5.7057913	3.3834107	-2.0415724
H	3.6260348	4.7981280	1.4624462
H	5.5863706	4.9033436	-0.0703689
C	0.7829445	-2.1283129	1.2232497
C	1.6841157	-2.9730700	1.8945266
C	-0.1273893	-2.6714268	0.3063602
C	1.6559131	-4.3484305	1.6658518
H	2.4227258	-2.5523944	2.5792812
C	-0.1383236	-4.0477914	0.0709044
H	-0.8006081	-2.0116445	-0.2472352
C	0.7453944	-4.8876541	0.7521509
H	2.3552406	-4.9988283	2.1944527
H	-0.8330270	-4.4619017	-0.6612807
H	0.7320119	-5.9628758	0.5648705
C	0.1287578	-0.1676453	3.2744449
C	-0.2083621	1.1187012	3.7313083
C	-0.0737107	-1.2624820	4.1268556
C	-0.7142621	1.3099810	5.0166643
H	-0.0739990	1.9682268	3.0569618
C	-0.5899955	-1.0705747	5.4124101
H	0.1654166	-2.2710156	3.7890648
C	-0.9073159	0.2128250	5.8622257
H	-0.9626570	2.3166200	5.3575680
H	-0.7409331	-1.9322529	6.0650262
H	-1.3026597	0.3583902	6.8689932
C	2.5753968	0.0659473	1.7253045
C	3.0533178	0.7065108	2.8796571
C	3.4404003	-0.1925923	0.6429339
C	4.3887302	1.0914194	2.9597353
H	2.3878546	0.8937557	3.7207107
C	4.7899928	0.2269881	0.7408685
C	5.2598702	0.8639010	1.8965309
H	4.7590747	1.5798451	3.8625323
H	6.2973880	1.1847716	1.9703130
O	5.5555746	-0.0082416	-0.3561435
O	4.3501140	-2.6935268	0.1101238
C	6.9247287	0.3920047	-0.3214102
H	7.3406680	0.1058030	-1.2935804
H	7.0185535	1.4824713	-0.1885680
H	7.4750023	-0.1273736	0.4799221
C	4.8999862	-3.9948857	-0.0868532
H	5.5313302	-4.1847053	0.7882330
H	4.1075164	-4.7595689	-0.1400519
H	5.5165234	-4.0372394	-0.9994626
C	-4.0978520	2.1065299	3.9118379
C	-3.8236805	3.2463135	3.2147606
C	-3.2925781	1.4924718	1.8970703
N	-3.7733376	1.0451431	3.0869060
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H	-3.9481438	4.2891964	3.4809780
N	-3.3330831	2.8479169	1.9840230
C	-2.9022899	3.7386711	0.9049166
H	-3.2623422	4.7453059	1.1686984
H	-3.4094809	3.4370332	-0.0225864
C	-1.4143894	3.7706729	0.6968784
H	-0.7969182	3.8699866	1.5946775
C	-0.8613581	3.8474055	-0.5236435
H	-1.4639379	3.7806256	-1.4323192
H	0.2031551	4.0299568	-0.6556953
C	-3.8612018	-0.3634809	3.4521781
B	-2.7613990	0.6105921	0.6989367
H	-3.4404317	-0.3841910	0.5529903
H	-2.6292855	1.2391938	-0.3454389
H	-1.6781323	0.0254794	1.1022423
H	-2.8604545	-0.7570708	3.6739413
H	-4.4966348	-0.4605154	4.3388546
H	-4.2936359	-0.9274210	2.6176028
H	-1.9111475	-1.2894987	-1.9710714
B	-2.7741132	-1.7101161	-2.7446755

H	-2.6122979	-1.2360635	-3.8601493
C	-4.1832690	-1.3814182	-2.0774067
C	-2.9114890	-3.3676488	-2.6904516
N	-4.6936889	-2.4453510	-1.4174651
N	-5.0706105	-0.3757137	-1.8897665
C	-3.5138972	-3.9448384	-3.9769432
H	-1.9382697	-3.8495047	-2.5065896
C	-3.8368086	-3.6435280	-1.4830792
C	-5.8804278	-2.1254541	-0.7929387
C	-6.1245344	-0.8127654	-1.0954367
C	-4.9150337	0.9634369	-2.4295105

H	-2.8584988	-3.7390573	-4.8345725
H	-4.4880382	-3.4799451	-4.2031355
H	-3.6701275	-5.0358340	-3.9213629
H	-4.4703049	-4.5388765	-1.5871323
H	-3.2772888	-3.7180513	-0.5360122
H	-6.4627315	-2.8364396	-0.2188411
H	-6.9591370	-0.1713957	-0.8362545
H	-3.9850440	0.9901889	-3.0067734
H	-5.7603429	1.2153175	-3.0842221
H	-4.8503363	1.6954458	-1.6128886