

Supporting information belonging to the paper

Propagation & Termination Steps in Rh-mediated Carbene Polymerisation using Diazomethane

Nicole M. G. Franssen,^{a,b} Markus Finger,^{a,b} Joost N. H. Reek,^a and Bas de Bruin^{*,a}

^a Van 't Hoff Institute for Molecular Sciences (HIMS), Department of Homogeneous and Supramolecular Catalysis, Universiteit van Amsterdam, P.O. Box 94720, 1090 GS Amsterdam, The Netherlands. Fax: +31 20 525 5604; Tel: +31 20 525 6495; E-mail: b.debruin@uva.nl.

^b Dutch Polymer Institute DPI, P.O. Box 902, 5600 AX Eindhoven, The Netherlands.

Contents

	Pages
Tabulated energies for the reaction pathways described in the main paper	2-7
Cartesian Coordinates of the structures described in the main paper	8-31

Tabulated energies for the reaction pathways described in the main paper.

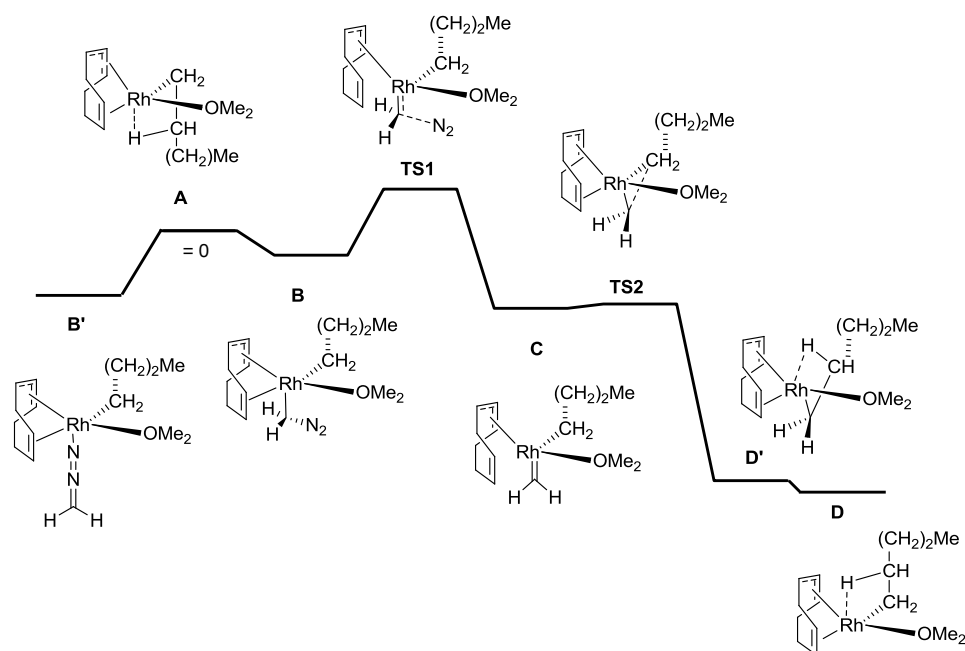


Figure S1. General representation of the calculated chain propagation pathway (b3-lyp, def2-TZVP) from complex A, involving carbene formation and carbene insertion into the Rh–C bond of the growing chain.

Table S1. Calculated energies for chain propagation from species A (b3-lyp, def2-TZVP) in kcal mol⁻¹ at 273 K.

Species	E _{scf}	E _{scf} + ZPE	ΔH^0	ΔG^0_{gas}	$\Delta G_{\text{solution}}^{\text{a}}$	$\Delta G_{\text{solution}}^{\text{b}}$
A	0	0	0	0	0	0
B	-6.4	-3.8	-3.8	+5.2	+2.7	-1.0
B'	-10.7	-8.7	-8.4	-0.9	-3.4	-7.1
TS1	+1.0	+2.6	+2.6	+11.9	+9.4	+5.7
C	-14.4	-14.7	-14.0	-14.1	-16.6	-20.3
TS2	-13.2	-13.1	-13.1	-11.4	-13.9	-17.6
D'	-58.6	-57.7	-57.5	-56.9	-59.3	-63.0
D	-60.4	-59.0	-58.9	-57.6	-60.1	-63.8

^a Corrected for the condensed-phase reference volume (2.5 kcal mol⁻¹ translational entropy correction).

^b Entropy factors corrected towards 'solution phase' values using a Trouton-like approach (6.2 kcal mol⁻¹ translational entropy correction).

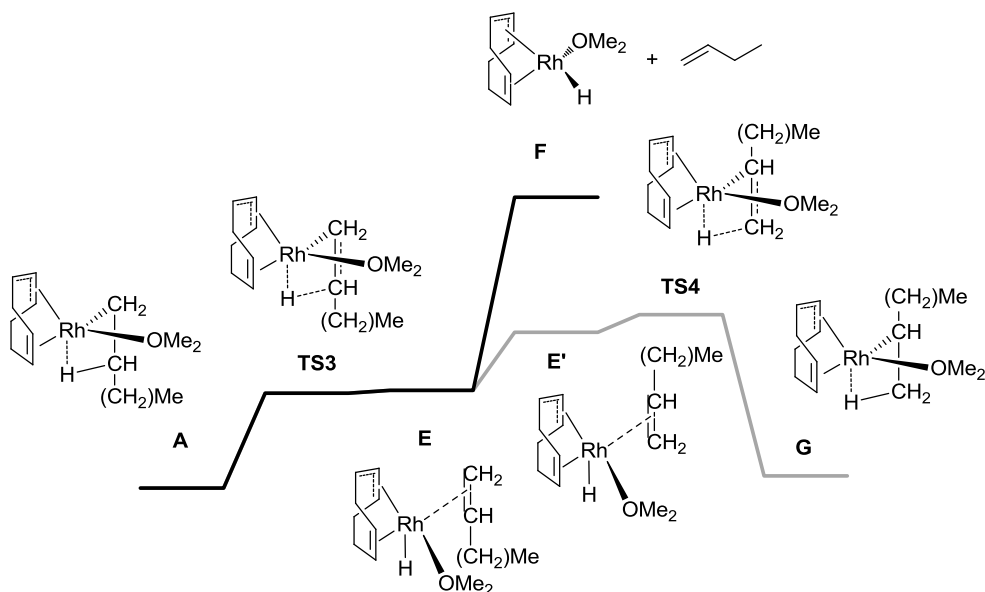


Figure S2. General representation of the calculated chain-termination pathway from complex **A** (b3-lyp, def2-TZVP) involving β -hydride elimination followed by alkene dissociation. The gray lines represent insertion of the alkene fragment after rotation to initiate the pathway leading to branched polymers.

Table S2. Calculated energies for chain termination from species **A** via β -hydride elimination followed by alkene dissociation (b3-lyp, def2-TZVP) in kcal mol⁻¹ at 273 K.

Species	E_{scf}	$E_{\text{scf}} + \text{ZPE}$	ΔH^0	ΔG^0	$\Delta G_{\text{solution}}^{\text{a}}$	$\Delta G_{\text{solution}}^{\text{b}}$
A	0	0	0	0	0	0
TS3	+8.0	+5.7	+5.7	+5.9	+5.9	+5.9
E^c	+7.3	+5.7	+6.0	+5.1	+5.1	+5.1
F + alkene	+20.3	+17.3	+17.5	+5.0	+7.5	+11.2
E'	+8.9	+7.4	+7.7	+7.1	+7.1	+7.1
TS4	+9.9	+7.6	+7.6	+7.6	+7.6	+7.6
F	+0.7	+0.6	+0.7	+0.9	+0.9	+0.9

^a Corrected for the condensed-phase reference volume (2.5 kcal mol⁻¹ translational entropy correction).

^b Entropy factors corrected towards 'solution phase' values using a Trouton-like approach (6.2 kcal mol⁻¹ translational entropy correction).

^c Since the number of species does not change from **A** via **TS3** to **E**, ΔG_{gas} equals $\Delta G_{\text{solution}}$.

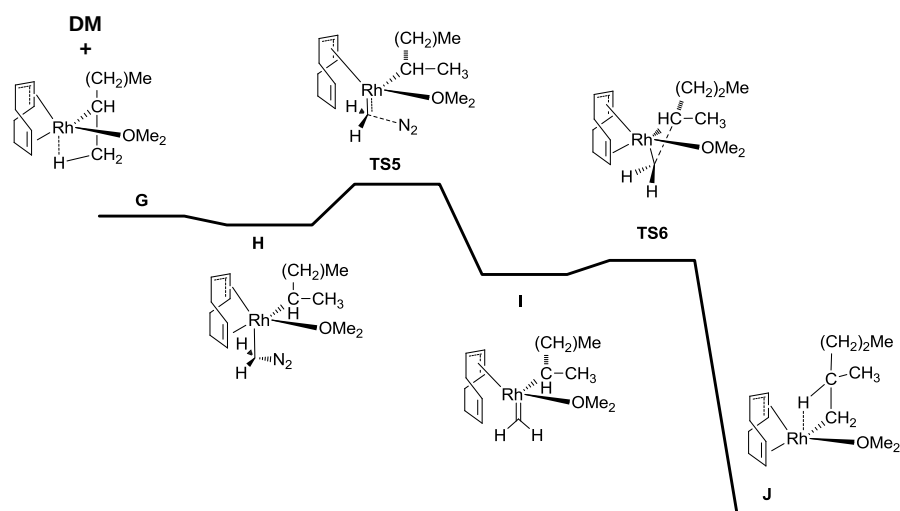


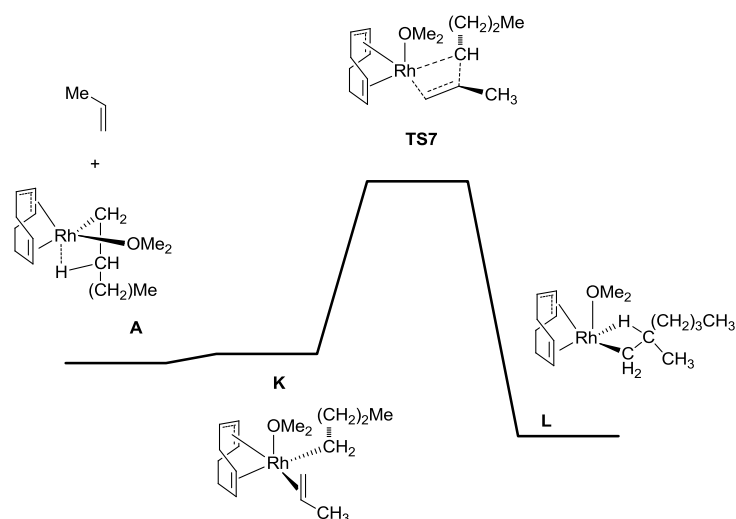
Figure S3. General representation of the calculated chain propagation pathway (b3-lyp, def2-TZVP) from complex **G** leading to branched polymers, involving carbene formation and carbene insertion into the Rh–C bond of the growing chain.

Table S3. Calculated energies for chain propagation from species **G** (b3-lyp, def2-TZVP) in kcal mol⁻¹ at 273 K.

Species	E_{scf}	$E_{\text{scf}} + \text{ZPE}$	ΔH^0	ΔG^0_{gas}	$\Delta G_{\text{solution}}^{\text{a}}$	$\Delta G_{\text{solution}}^{\text{b}}$
G	0	0	0	0	0	0
H	-4.1	-3.0	-3.0	+6.8	+4.3	+0.6
TS5	+3.6	+4.6	+4.9	+13.8	+11.3	+7.6
I	-12.5	-13.6	-12.7	-14.2	-16.7	-20.4
TS6	-8.7	-9.8	-9.2	-9.2	-11.7	-15.4
J	-60.5	-59.4	-59.3	-57.7	-60.2	-63.9

^a Corrected for the condensed-phase reference volume (2.5 kcal mol⁻¹ translational entropy correction).

^b Entropy factors corrected towards 'solution phase' values using a Trouton-like approach (6.2 kcal mol⁻¹ translational entropy correction).



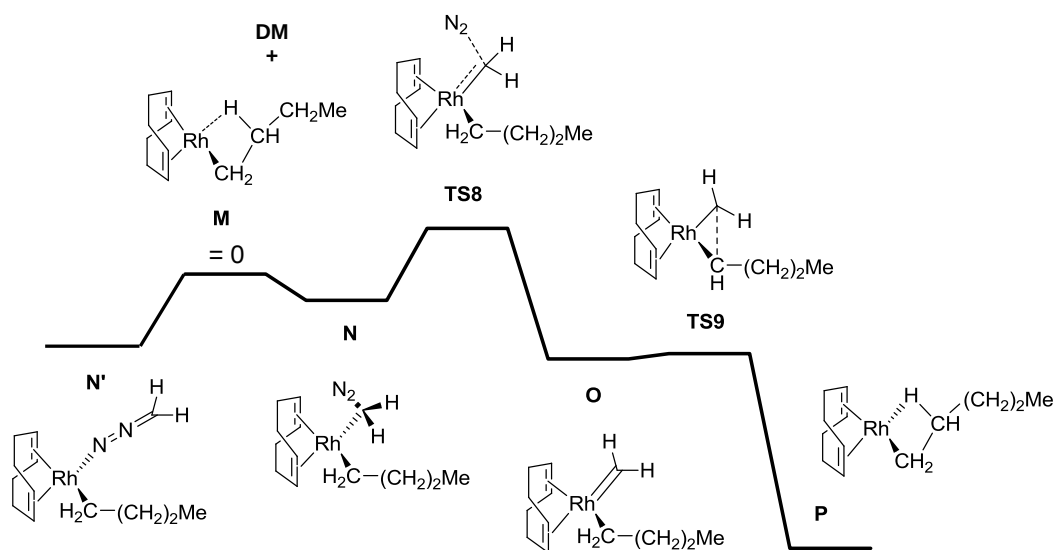
FigureS4. General representation of the calculated chain propagation pathway (b3-lyp, def2-TZVP) from complex **A** leading to branched polymers, involving propene insertion into the Rh–C bond of the growing chain.

Table S4. Calculated energies for propene insertion into the growing chain of species **A** (b3-lyp, def2-TZVP) in kcal mol⁻¹ at 273 K.

Species	E_{scf}	$E_{\text{scf}} + \text{ZPE}$	ΔH^0	ΔG^0_{gas}	$\Delta G^0_{\text{solution}}{}^{\text{a}}$	$\Delta G^0_{\text{solution}}{}^{\text{b}}$
A	0	0	0	0	0	0
K	-1.4	+1.0	+1.2	+10.6	+8.1	+4.4
TS7	+22.1	+23.8	+23.7	+32.6	+32.1	+26.4
L	-12.2	-9.0	-9.5	+1.5	-1.0	-4.7

^a Corrected for the condensed-phase reference volume (2.5 kcal mol⁻¹ translational entropy correction).

^b Entropy factors corrected towards 'solution phase' values using a Trouton-like approach (6.2 kcal mol⁻¹ translational entropy correction).



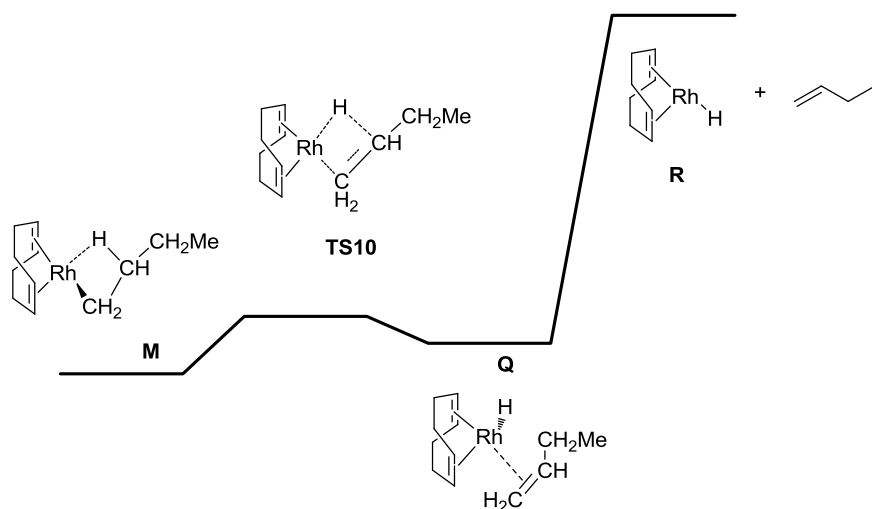
FigureS5. General representation of the calculated chain propagation pathway (b3-lyp, def2-TZVP) from complex **M**, involving carbene formation and carbene insertion into the Rh–C bond of the growing chain.

Table S5. Calculated energies for chain propagation from species **M** (b3-lyp, def2-TZVP) in kcal mol⁻¹ at 273 K.

Species	E _{scf}	E _{scf} + ZPE	ΔH ⁰	ΔG ⁰ _{gas}	ΔG ⁰ _{solution} ^a	ΔG ⁰ _{solution} ^b
M	0	0	0	0	0	0
N	-8.4	-6.0	-6.2	+3.9	+1.4	-2.3
N'	-13.8	-11.2	-11.2	-2.0	-5.5	-8.2
TS8	+8.5	+10.4	+10.0	+21.3	+18.8	+15.1
O	-19.0	-19.3	-18.5	-18.6	-21.1	-24.8
TS9	-17.2	-17.2	-17.1	-15.6	-18.1	-21.8
P	-60.2	-58.6	-58.6	-57.2	-59.7	-63.4

^a Corrected for the condensed-phase reference volume (2.5 kcal mol⁻¹ translational entropy correction).

^b Entropy factors corrected towards 'solution phase' values using a Trouton-like approach (6.2 kcal mol⁻¹ translational entropy correction).



FigureS6. General representation of the calculated chain-termination pathway from complex **M** (b3-lyp, def2-TZVP) involving β -hydride elimination followed by alkene dissociation.

Table S6. Calculated energies for chain termination from species **M** via β -hydride elimination followed by alkene dissociation (b3-lyp, def2-TZVP) in kcal mol⁻¹ at 273 K.

Species	E_{scf}	$E_{\text{scf}} + \text{ZPE}$	ΔH^0	ΔG_{gas}^0	$\Delta G_{\text{solution}}^{\text{a}}$	$\Delta G_{\text{solution}}^{\text{b}}$
M	0	0	0	0	0	0
TS10	+5.2	+3.4	+3.2	+3.9	+3.9 ^c	+3.9^c
Q	+2.4	+1.7	+1.7	+2.0	+2.0 ^c	+2.0^c
R + alkene	+22.4	-19.9	+20.0	+8.5	+11.0	+14.7

^a Corrected for the condensed-phase reference volume (2.5 kcal mol⁻¹ translational entropy correction).

^b Entropy factors corrected towards 'solution phase' values using a Trouton-like approach (6.2 kcal mol⁻¹ translational entropy correction).

^c Since the number of species does not change from **M** via **TS10** to **Q**, ΔG_{gas} equals $\Delta G_{\text{solution}}$.

Cartesian Coordinates of the structures described in the main paper.

A

Rh	-0.6820484	0.4774438	1.7317696
C	-0.1654592	2.742547	0.7704869
H	-0.1583652	3.4617762	1.5850012
C	-1.3910582	2.3670526	0.3307183
H	-2.2457504	2.7927384	0.8431232
C	-0.4611179	-0.708208	-0.0120331
C	0.7793503	-0.0612711	0.2673579
C	-1.6413364	0.0199138	-0.233395
H	-2.5621486	-0.5520299	-0.2092406
H	-0.5614577	-1.7687299	0.1868953
H	1.538676	-0.720811	0.6776568
C	-1.7330973	1.4244618	-0.8071353
H	-1.095645	1.5593379	-1.6790769
H	-2.7540912	1.6132762	-1.1353761
C	1.1921155	2.4707854	0.1740908
H	1.9300264	2.551253	0.9754565
H	1.4350333	3.2766388	-0.528235
C	1.3481841	1.1152722	-0.5236488
H	2.4115884	0.9321177	-0.6864042
H	0.8989796	1.1414447	-1.5149877
H	0.3989239	0.9119253	3.2404195
C	0.5397316	-0.159801	3.7020839
H	1.6073247	-0.3165371	3.541835
C	-0.2919437	-1.1297234	2.9305037
H	0.2427851	-1.946454	2.4547756
O	-2.4696496	0.9380503	3.1533968
C	-2.6669733	2.2187438	3.7624498
H	-1.6905498	2.6786966	3.8932727
H	-3.1427054	2.0951304	4.7384138
H	-3.2955047	2.8576118	3.1353144
C	-3.7013102	0.2221311	2.9924081
H	-4.358876	0.7409422	2.2883903
H	-4.2059559	0.1290932	3.9571436
H	-3.4597039	-0.7664897	2.6117793
H	-1.1909054	-1.477155	3.4352189
C	0.2171547	0.0262323	5.1890652
H	0.4312187	-0.9256941	5.6833678
H	-0.8560273	0.1958627	5.303121
C	1.0129298	1.145341	5.8540194
H	2.0881628	0.9677277	5.7807273
H	0.7645111	1.2217416	6.9131813
H	0.8042464	2.1165061	5.3962923

B

C	-0.2011665	2.3602418	0.0082711
H	-0.4930577	3.3424888	0.3704028
C	-1.2113273	1.5748145	-0.4165558
H	-2.2132278	1.9776739	-0.3261268
C	0.0769418	-1.1034853	0.865532
C	1.1139151	-0.1452804	1.1107664
C	-1.0544793	-0.8202496	0.1034257
H	-1.8650792	-1.5376818	0.1646418
H	0.0555678	-2.00394	1.4647612
H	1.80899	-0.4471707	1.8888022
C	-1.1357428	0.1925154	-1.0265934
H	-0.3018651	0.0898915	-1.7202964
H	-2.041156	0.0103291	-1.6037542

C	1.2861271	2.1471831	-0.0851238
H	1.7603095	2.7332882	0.7070086
H	1.6492317	2.5907469	-1.0196039
C	1.7654682	0.6939673	0.0074342
H	2.8431308	0.7031291	0.179203
H	1.6282012	0.1928614	-0.9502547
C	-1.5205507	-2.7732825	4.7491417
Rh	-0.7179835	0.5995829	1.8841584
H	-0.5427926	-3.2464698	4.6112198
H	-2.2618467	-3.569786	4.6369176
O	-2.9546492	1.3705685	2.3646691
N	-0.6229474	2.4217725	4.2981206
N	-1.3451788	2.5860163	5.1199378
C	0.1809776	2.1249688	3.2214266
H	0.3791664	3.060388	2.7015122
H	1.0888402	1.6703363	3.6134943
C	-3.3093809	2.7532968	2.30817
H	-2.4046294	3.343935	2.4267217
H	-4.0135056	2.9963443	3.1083484
H	-3.7668968	2.9999081	1.3450807
C	-4.0954499	0.5435956	2.0965771
H	-4.5125969	0.780087	1.1127479
H	-4.8615522	0.7035009	2.8597493
H	-3.76896	-0.4897639	2.1173482
C	-1.7506302	-1.751945	3.6152701
H	-2.7324239	-1.2952436	3.7652793
H	-1.8045506	-2.3053265	2.6727247
C	-0.6795867	-0.6710372	3.5492819
H	0.3169832	-1.1198048	3.5846597
H	-0.7713665	-0.0242911	4.4223817
C	-1.6191564	-2.1939997	6.1599296
H	-0.8366204	-1.4591989	6.3599921
H	-1.520671	-2.9814007	6.9087791
H	-2.5854385	-1.7077013	6.320536

B'

C	-0.4976263	2.3035439	-0.2550028
H	-0.8559609	3.2777696	0.0641771
C	-1.4496601	1.4220004	-0.6186207
H	-2.4764778	1.7612937	-0.5437733
C	0.0443027	-1.0944702	0.8164079
C	1.0052353	-0.0500713	0.9901542
C	-1.118845	-0.9275252	0.0590244
H	-1.8699296	-1.7014422	0.1694955
H	0.0948275	-1.9589438	1.4650169
H	1.7185389	-0.2394552	1.7869035
C	-1.2822431	0.0060597	-1.1319542
H	-0.4516181	-0.0864374	-1.8309149
H	-2.1788422	-0.2767458	-1.6822454
C	1.0006777	2.187312	-0.3189611
H	1.4155065	2.8363877	0.4568971
H	1.3476497	2.6179402	-1.2655958
C	1.5800288	0.7768337	-0.1631292
H	2.6564066	0.8686665	-0.007171
H	1.467629	0.2201445	-1.0928494
C	-1.6992705	-2.4393651	4.9142007
Rh	-0.8885858	0.5845251	1.7287288
H	-0.681269	-2.819052	5.0460704
H	-1.8675374	-1.7239111	5.7250671
O	-3.1465924	1.1061102	2.2619991

N	0.4819974	2.4140885	3.6605869
N	-0.3390394	2.2196394	2.8780883
C	1.3737093	2.6712285	4.5305731
H	1.1243344	2.5514516	5.5752278
H	2.3410166	3.0169388	4.1950077
C	-3.5649592	2.4126946	2.6736786
H	-2.7208643	2.897974	3.1531211
H	-4.3926928	2.329003	3.3820644
H	-3.8863923	3.005586	1.8116319
C	-4.2216927	0.3820668	1.6555804
H	-4.5493853	0.8731562	0.7339414
H	-5.0665142	0.3210002	2.3463501
H	-3.8649542	-0.6191701	1.4337752
C	-1.7928902	-1.7029213	3.5651693
H	-2.8136353	-1.3310118	3.446749
H	-1.6288632	-2.4308452	2.7645232
C	-0.8049661	-0.5531884	3.4758676
H	0.2243043	-0.9001244	3.5974166
H	-1.0129257	0.1707979	4.2666786
C	-2.6970571	-3.5906221	5.0300829
H	-2.6075451	-4.0908569	5.9958906
H	-2.5302607	-4.3403682	4.2525941
H	-3.7265732	-3.235566	4.9358487

TS1

C	-0.1751217	2.3876032	0.0420605
H	-0.464221	3.3522821	0.4494948
C	-1.1814043	1.6285617	-0.433149
H	-2.1852808	2.0247156	-0.3352082
C	0.0320598	-1.1107211	0.7383549
C	1.0726927	-0.1690064	1.0894893
C	-1.0300485	-0.818349	-0.0854544
H	-1.8409099	-1.5383288	-0.1047922
H	-0.0265232	-2.0338461	1.3008662
H	1.7526656	-0.547113	1.8467431
C	-1.0878277	0.2884759	-1.1234915
H	-0.232837	0.2374925	-1.7977022
H	-1.9740236	0.146648	-1.7404583
C	1.3114867	2.158606	-0.040936
H	1.7814418	2.7266575	0.7666493
H	1.6910788	2.6136805	-0.9631796
C	1.7769983	0.6980457	0.0364825
H	2.8464461	0.6972013	0.2529532
H	1.6785473	0.2199702	-0.9380346
C	-1.6251161	-2.6779137	4.7655241
Rh	-0.6992718	0.6109526	1.9085152
H	-0.7462663	-3.2868865	4.5325758
H	-1.4052354	-2.1742021	5.71215
O	-3.0056826	1.2993724	2.3289722
N	-0.7830834	2.3752689	4.5145556
N	-1.5686712	2.4397119	5.2731861
C	0.1998078	1.9384096	3.0903747
H	0.3511575	2.9729695	2.778312
H	1.0452731	1.6105967	3.6962765
C	-3.3687254	2.6805696	2.2905031
H	-2.4810501	3.2713233	2.5009638
H	-4.1351243	2.8909673	3.041394
H	-3.7541207	2.9569425	1.3042026
C	-4.1165032	0.4701506	1.9633759
H	-4.4482268	0.7043373	0.9470217

H	-4.9465349	0.6278278	2.6572109
H	-3.7915358	-0.5630847	2.0158564
C	-1.8103169	-1.6194321	3.6634677
H	-2.6989834	-1.028167	3.9005646
H	-2.0195792	-2.1379026	2.7204369
C	-0.5992688	-0.7099047	3.529091
H	0.3139385	-1.2967686	3.4114439
H	-0.4785917	-0.1302698	4.4455489
C	-2.8474942	-3.5786452	4.933988
H	-2.683123	-4.3193442	5.7180093
H	-3.0737706	-4.1194622	4.0114814
H	-3.733434	-2.9997499	5.2068781
<u>C</u>			
C	-0.1933558	2.386407	-0.0112505
H	-0.4578471	3.3537596	0.4063443
C	-1.2114946	1.6410809	-0.4750947
H	-2.2124718	2.044687	-0.3693983
C	-0.1238488	-1.1242847	0.6569157
C	0.9226499	-0.1997558	1.0932115
C	-1.0738856	-0.8662569	-0.2782503
H	-1.8456656	-1.6163994	-0.416002
H	-0.2085251	-2.0582303	1.1990019
H	1.5792416	-0.6534119	1.8279511
C	-1.1222335	0.3242245	-1.2133565
H	-0.2550167	0.3098664	-1.8769763
H	-1.9964439	0.2279235	-1.8563277
C	1.2823361	2.1038804	-0.099374
H	1.7823466	2.7011483	0.6660372
H	1.6647584	2.49036	-1.0510044
C	1.7023377	0.633142	0.0604853
H	2.7563551	0.6172816	0.3411377
H	1.6492298	0.1191463	-0.9000963
C	-1.6564547	-2.5382082	4.8767042
Rh	-0.713397	0.7213155	2.0175173
H	-0.7048728	-3.0709879	4.7872498
H	-1.6041808	-1.9717761	5.8114225
O	-2.9725088	1.1360347	2.38781
C	0.2542296	1.8970704	3.0409273
H	0.6483499	2.8313654	2.6342646
H	0.5440075	1.7346861	4.0807619
C	-3.3621423	2.4740942	2.7374078
H	-2.5978491	2.8766915	3.3957187
H	-4.3194257	2.4487463	3.2615102
H	-3.4531108	3.0988315	1.8442145
C	-4.016765	0.4378589	1.693985
H	-4.2218446	0.9075086	0.7273323
H	-4.9256874	0.4447354	2.2991987
H	-3.6886669	-0.5873069	1.549042
C	-1.7987241	-1.5551851	3.6985929
H	-2.7556465	-1.0374507	3.7927568
H	-1.8423059	-2.1373354	2.7723268
C	-0.6601184	-0.5489373	3.6726817
H	0.312236	-1.0447389	3.6706934
H	-0.7098178	0.092276	4.5536005
C	-2.8058236	-3.5424104	4.946292
H	-2.6753417	-4.2268388	5.785768
H	-2.8648215	-4.1439182	4.0358338
H	-3.7667125	-3.0388764	5.0769644

TS2

C	0.0529051	2.1638071	0.2015261
H	0.049085	3.0990239	0.7515116
C	-1.1175889	1.8229748	-0.4157328
H	-1.9643424	2.4846762	-0.275962
C	-0.9190779	-1.1899525	0.2975018
C	0.3205215	-0.6525303	0.8528144
C	-1.7174489	-0.549527	-0.6063042
H	-2.6852761	-0.989528	-0.8182945
H	-1.3156211	-2.096287	0.7408586
H	0.7581328	-1.3009674	1.6044405
C	-1.3377389	0.6904947	-1.3934837
H	-0.4655017	0.5157077	-2.0236802
H	-2.155906	0.956479	-2.0607334
C	1.4072562	1.5283825	0.0133392
H	2.0401771	1.8471325	0.8424176
H	1.8699988	1.941725	-0.8905315
C	1.3814504	-0.0046569	-0.0528524
H	2.3631903	-0.3812785	0.2358431
H	1.2293177	-0.3431826	-1.0782753
C	-1.7273856	-2.7673713	4.7564437
Rh	-1.0839185	0.6484471	1.6599999
H	-2.2327119	-2.195266	5.5407819
H	-2.5187666	-3.2115222	4.1434333
O	-2.9825435	1.9780774	2.33476
C	-0.2753574	1.07856	3.2723421
H	0.7191694	0.7495966	3.5763227
H	-0.7965679	1.627043	4.059587
C	-2.8972098	3.3930291	2.5240036
H	-1.8733512	3.6292526	2.8045169
H	-3.5729835	3.7063634	3.3237536
H	-3.1591885	3.9281494	1.6055032
C	-4.3131714	1.5593209	2.0126987
H	-4.6290993	1.9765172	1.0514864
H	-5.0081279	1.8830203	2.7916344
H	-4.3131173	0.4738754	1.9585747
C	-0.8971011	-1.8069398	3.8878107
H	-0.3957189	-2.3886346	3.1090061
H	-0.1043237	-1.3737135	4.5063657
C	-1.7651339	-0.7232562	3.2797476
H	-2.253561	-0.1145948	4.0374906
H	-2.5462025	-1.1471165	2.6467371
C	-0.8837418	-3.8734057	5.3883739
H	-1.5005647	-4.529779	6.0036336
H	-0.1007062	-3.4597227	6.0283748
H	-0.4010765	-4.4906109	4.6267451

D'

C	0.2257606	1.8478254	0.5489388
H	0.3576852	2.7002684	1.2068879
C	-0.9300049	1.8499841	-0.214094
H	-1.6082249	2.6825659	-0.065853
C	-1.3536393	-1.1872036	-0.028972
C	-0.1006746	-0.9407276	0.6830857
C	-1.9257703	-0.292812	-0.885201
H	-2.9199138	-0.5164837	-1.2552472
H	-1.9377073	-2.061524	0.2389845
H	0.1257145	-1.7112623	1.4152336
C	-1.2611342	0.972705	-1.4028348
H	-0.3877997	0.7448126	-2.0162204

H	-1.9599386	1.5029094	-2.0482215
C	1.4675569	1.0203422	0.3165818
H	2.0615985	1.0466207	1.2313604
H	2.0839675	1.4980466	-0.4537095
C	1.1497411	-0.4316197	-0.0496192
H	1.9979095	-1.0665677	0.2093964
H	1.0151342	-0.5431911	-1.1250643
C	-1.4039149	-2.6260554	4.5595625
Rh	-1.3057476	0.5217696	1.5172254
H	-2.2806929	-2.3773731	5.1667743
H	-1.7892778	-2.941355	3.5823728
O	-3.1758093	1.875531	2.219058
C	-0.48539	0.9906418	3.3511306
H	0.5942078	0.8808812	3.3878967
H	-0.8166059	1.9588583	3.7134505
C	-3.1412538	3.2963662	2.3757478
H	-2.1169087	3.5820302	2.6028354
H	-3.791471	3.5995639	3.2003797
H	-3.4688438	3.7979629	1.4596852
C	-4.4978397	1.3993443	1.9431717
H	-4.857488	1.7874089	0.9854649
H	-5.1819479	1.7081504	2.7378103
H	-4.4556855	0.3134443	1.9040592
C	-0.5410201	-1.3761768	4.3861996
H	0.34034	-1.6066536	3.7801619
H	-0.1610252	-1.0552984	5.3611696
C	-1.2805503	-0.1816234	3.7835952
H	-2.1538501	0.1054454	4.37212
H	-1.8457797	-0.6362895	2.8352607
C	-0.6470241	-3.7849585	5.2053673
H	-1.2897804	-4.6588042	5.3181044
H	-0.2806653	-3.5133415	6.1978858
H	0.2148358	-4.0823447	4.6026089

D			
Rh	-0.6838854	0.4659467	1.710374
C	-0.1634198	2.7296857	0.7569465
H	-0.138018	3.4427734	1.576521
C	-1.398753	2.3678682	0.3326933
H	-2.241987	2.7970056	0.8609829
C	-0.5013518	-0.7121846	-0.044126
C	0.7489987	-0.0776941	0.2210366
C	-1.6780229	0.0271641	-0.2442219
H	-2.6034442	-0.5367871	-0.210144
H	-0.6079896	-1.7729691	0.1502666
H	1.5085577	-0.7467671	0.6152492
C	-1.7658683	1.4366432	-0.8067321
H	-1.1401485	1.5723543	-1.6869359
H	-2.7899196	1.636745	-1.1183693
C	1.182647	2.4509152	0.1379202
H	1.9331136	2.5191249	0.9288248
H	1.4218897	3.25973	-0.5622718
C	1.3162976	1.0988492	-0.5713519
H	2.375449	0.9076399	-0.7516651
H	0.852179	1.1355978	-1.5555236
H	0.4230702	0.8880823	3.1928679
C	0.5626282	-0.1861635	3.6549898
H	1.6238099	-0.3534987	3.47514
C	-0.287761	-1.1497413	2.8967757
H	0.2328383	-1.9682761	2.4086282

O	-2.4479622	0.9301086	3.1578968
C	-2.619105	2.206621	3.783529
H	-1.6334448	2.6445845	3.9195349
H	-3.0962661	2.0799441	4.7583059
H	-3.2351096	2.8660463	3.1654247
C	-3.6926823	0.2390174	2.9907632
H	-4.3396912	0.7749931	2.2900726
H	-4.1996529	0.1486328	3.9542839
H	-3.4691862	-0.751292	2.6034011
H	-1.1817845	-1.491322	3.4140069
C	0.250398	0.007168	5.1438878
H	0.4957267	-0.9343757	5.6461952
H	-0.827557	0.1440238	5.2583344
C	1.0001344	1.1592161	5.8201564
H	0.6039287	1.2701595	6.8329068
H	0.7677714	2.0993785	5.3045096
C	2.5166893	0.9770118	5.8966893
H	2.9786211	1.802079	6.4407814
H	2.9825903	0.9426653	4.9090675
H	2.7750664	0.0523064	6.4186707

TS3

Rh	-0.6204622	0.5319963	1.8029338
C	-0.1823567	2.6617411	0.8713288
H	-0.2186721	3.3654859	1.6960153
C	-1.3929119	2.2278869	0.4033886
H	-2.2756551	2.5885404	0.9176345
C	-0.4245932	-0.6940045	-0.0793481
C	0.7835152	-0.0134373	0.3584868
C	-1.5682501	-0.0485724	-0.4725293
H	-2.4565928	-0.6547173	-0.6087739
H	-0.4971838	-1.7648038	0.0734962
H	1.5315409	-0.6931746	0.7578364
C	-1.6696496	1.4195942	-0.8454207
H	-1.0011543	1.6736668	-1.6681074
H	-2.6800964	1.6341384	-1.189947
C	1.1701717	2.5136424	0.2174766
H	1.9278118	2.6827099	0.9838375
H	1.3025939	3.3171121	-0.5163274
C	1.4009575	1.1467537	-0.4351525
H	2.4742597	0.9755127	-0.5275056
H	1.0135765	1.1342046	-1.4536134
H	0.2727133	1.2522261	2.8893127
C	0.5289252	-0.3554993	3.6276951
H	1.5798864	-0.332464	3.3557624
C	-0.2848835	-1.2695991	2.943951
H	0.1763332	-2.0062853	2.2990845
O	-2.542369	0.8905874	3.1663746
C	-2.8045145	2.1395026	3.8129485
H	-1.8474797	2.6107152	4.0214073
H	-3.3386651	1.9695763	4.7514581
H	-3.4070236	2.7926913	3.1741922
C	-3.7460244	0.1642511	2.8951632
H	-4.3769939	0.7097935	2.186733
H	-4.302856	0.0022827	3.8217116
H	-3.4632629	-0.7948896	2.4691688
H	-1.2201947	-1.5757722	3.4000254
C	0.2334554	0.1232275	5.0267732
H	0.5330786	-0.7094398	5.6763391
H	-0.8441304	0.232947	5.1601691

C	0.9807709	1.3805974	5.4603354
H	2.060996	1.2560591	5.3586793
H	0.7731331	1.6097122	6.5058211
H	0.6883039	2.2496259	4.8653789

E

Rh	-0.6180429	0.5586032	1.8322645
C	-0.2372963	2.6535049	0.8729828
H	-0.3146545	3.372905	1.680648
C	-1.4252898	2.1570197	0.3969743
H	-2.3288522	2.4890374	0.8942879
C	-0.3675821	-0.70189	-0.0996203
C	0.7964035	0.0217691	0.4118428
C	-1.5024227	-0.1085944	-0.5657338
H	-2.3484735	-0.7490134	-0.7878828
H	-0.3974297	-1.7786279	0.0229365
H	1.549559	-0.6428809	0.8271026
C	-1.6522491	1.3684604	-0.8747425
H	-0.9802341	1.6755205	-1.6774726
H	-2.6639715	1.5607036	-1.2291542
C	1.1240752	2.5549815	0.2300438
H	1.8668835	2.7782822	0.9965264
H	1.2212237	3.3465235	-0.5222447
C	1.4171309	1.1824231	-0.3839306
H	2.4971154	1.03886	-0.4322239
H	1.0690366	1.1375603	-1.4161669
H	0.1950189	1.430392	2.8233567
C	0.4605113	-0.5308871	3.6297498
H	1.5064392	-0.5006225	3.3424993
C	-0.3762331	-1.3701929	2.924051
H	0.0306272	-2.0679332	2.205625
O	-2.5580505	0.9245361	3.1798395
C	-2.7575871	2.1419547	3.9047148
H	-1.7779252	2.5359788	4.1616075
H	-3.3221781	1.9441865	4.8195497
H	-3.3042481	2.8722665	3.2998886
C	-3.7957219	0.2879094	2.8466089
H	-4.386654	0.9140505	2.1709374
H	-4.3745543	0.0942784	3.7534737
H	-3.5607126	-0.6546261	2.3584478
H	-1.3487361	-1.6234915	3.3316539
C	0.16187	-0.0157549	5.0109035
H	-0.9163135	0.0717953	5.1503546
H	0.5973817	0.9755386	5.1503133
C	0.7492015	-0.9746207	6.0609061
H	1.8295264	-1.0793534	5.9451481
H	0.3025623	-1.9672081	5.984747
H	0.5567001	-0.5916556	7.0636822

E'

Rh	-0.7334513	0.6490664	1.9807313
C	-0.449298	2.6176761	0.7456372
H	-0.6524417	3.4312041	1.4332059
C	-1.5487471	1.9569111	0.2596805
H	-2.51463	2.2714422	0.6358942
C	-0.2276475	-0.8422352	0.2721687
C	0.8276044	0.0463888	0.7570591
C	-1.3615364	-0.4210722	-0.3563626
H	-2.1336246	-1.1588725	-0.5426557
H	-0.1833429	-1.8906481	0.5423823

H	1.5936405	-0.4822031	1.318325
C	-1.6002048	0.9772777	-0.8924196
H	-0.8873619	1.227228	-1.67916
H	-2.5895567	1.0232002	-1.3455438
C	0.967036	2.5502875	0.230759
H	1.620007	2.9429434	1.011068
H	1.0690218	3.2345226	-0.6196444
C	1.4184169	1.1369286	-0.1521238
H	2.5064663	1.0871906	-0.1004039
H	1.1638538	0.9166989	-1.1893055
H	-0.0856897	1.7387353	2.8690934
C	0.1766669	-0.0673455	3.9274026
H	1.2374046	0.1232088	3.8418118
C	-0.3900862	-1.1851569	3.355092
H	0.2626853	-1.8228605	2.7674352
O	-2.7716048	1.1836681	3.1645612
C	-2.8556878	2.3487145	3.9927704
H	-1.8563309	2.5685615	4.3584572
H	-3.5214192	2.1594478	4.8387381
H	-3.234243	3.2035426	3.4234962
C	-4.0586169	0.7775153	2.6895679
H	-4.5058996	1.5541993	2.061102
H	-4.7251871	0.5769106	3.5324802
H	-3.9257639	-0.132013	2.1100452
H	-0.3252457	0.4415429	4.7412348
C	-1.6444476	-1.8499363	3.8584436
H	-1.3354087	-2.4479574	4.7258623
H	-2.3354071	-1.0994574	4.2451971
C	-2.3356243	-2.7768684	2.8592184
H	-1.6538959	-3.5525787	2.5026192
H	-2.709858	-2.235276	1.9884101
H	-3.1832154	-3.2786442	3.3266716

F

Rh	-1.5262051	1.7393879	1.3780998
C	-0.2901792	3.0388119	0.0788506
H	-0.4694564	4.0694551	0.3629264
C	-1.2924178	2.4361055	-0.6678868
H	-2.177516	3.0366378	-0.8598639
C	-0.917379	-0.3765725	0.51445
C	0.0754064	0.4699137	1.1878791
C	-1.533535	-0.0364658	-0.6456014
H	-2.3281964	-0.6831924	-1.0018075
H	-1.2728539	-1.2577638	1.0374307
H	0.3365492	0.1096237	2.1801441
C	-1.1920502	1.1711966	-1.500991
H	-0.2071456	1.0568469	-1.9593221
H	-1.9052122	1.2370998	-2.3213317
C	1.1377656	2.5761074	0.2380405
H	1.5529965	3.0858124	1.1082155
H	1.7271058	2.9145789	-0.6213172
C	1.2624145	1.0575389	0.4171803
H	2.1825224	0.8306435	0.9566998
H	1.3463025	0.5586172	-0.5479355
H	-1.1688264	2.9759631	2.2411513
O	-2.25509	0.7267402	3.1552091
C	-1.7315165	1.0779427	4.4548925
H	-0.6544418	1.1722152	4.3564661
H	-1.9738198	0.280905	5.159514
H	-2.1595275	2.0236609	4.7928764

C	-3.6759696	0.4835296	3.1869059
H	-4.2151313	1.3929281	3.4633889
H	-3.886567	-0.3065984	3.9094791
H	-3.974584	0.1556927	2.1932515

TS4

Rh	-0.7775403	0.5765033	1.9379273
C	-0.3873663	2.6385708	0.8020449
H	-0.544764	3.4214038	1.5363054
C	-1.5178986	2.0746544	0.2814467
H	-2.4653374	2.4247629	0.6732303
C	-0.3316991	-0.8211001	0.2286618
C	0.7870081	-0.0169621	0.6876732
C	-1.4727108	-0.2968641	-0.3235598
H	-2.3091896	-0.9725341	-0.461203
H	-0.3549244	-1.8721659	0.491316
H	1.5359478	-0.5949855	1.2221536
C	-1.6247435	1.1085134	-0.8782576
H	-0.897379	1.3129401	-1.6635414
H	-2.6088614	1.2091231	-1.3335583
C	1.0308784	2.5061389	0.3036581
H	1.6960322	2.8014764	1.1165166
H	1.196597	3.2354924	-0.497713
C	1.4011793	1.0971395	-0.1713429
H	2.4867506	0.9934714	-0.1524172
H	1.1116416	0.9514382	-1.2121171
H	-0.0607945	1.4887816	3.0069923
C	0.1901425	0.0291715	3.8862097
H	1.260918	0.1798061	3.8407531
C	-0.3840487	-1.1120424	3.3040778
H	0.2956984	-1.7665626	2.7662052
O	-2.8033882	1.1241491	3.1049901
C	-2.9113813	2.3361232	3.8591814
H	-1.9215908	2.5853931	4.2326772
H	-3.5930464	2.1921772	4.7011218
H	-3.283134	3.1534992	3.2332327
C	-4.078816	0.6799684	2.6300139
H	-4.5093735	1.4062042	1.9333091
H	-4.7649001	0.5422189	3.4696936
H	-3.930016	-0.2700903	2.1247684
H	-0.2924024	0.4820335	4.7453145
C	-1.5841715	-1.8139395	3.8928381
H	-1.2240684	-2.3522323	4.7792252
H	-2.3032741	-1.0805067	4.2606136
C	-2.2562413	-2.8205759	2.9601419
H	-1.5473796	-3.5797084	2.6210953
H	-2.6787528	-2.3403102	2.0751452
H	-3.0662716	-3.3386868	3.4741789

G

Rh	-0.8570465	0.4819987	1.854178
C	-0.3621442	2.7333274	0.7421052
H	-0.4768948	3.5200651	1.4828825
C	-1.5117281	2.2505982	0.2182718
H	-2.4351193	2.6696671	0.6013051
C	-0.3956796	-0.8040916	0.2353192
C	0.7743087	-0.0684162	0.5818838
C	-1.5839436	-0.1589596	-0.1486131
H	-2.4717541	-0.7810809	-0.1729152
H	-0.4603753	-1.8524657	0.5002943

H	1.5239254	-0.6511467	1.1095557
C	-1.6876119	1.186922	-0.8489162
H	-0.9738889	1.2841236	-1.6654424
H	-2.6780389	1.2847287	-1.2912107
C	1.0649507	2.4757774	0.3328893
H	1.6985406	2.6495993	1.2058842
H	1.3622236	3.237438	-0.3973874
C	1.3570809	1.0830743	-0.2352341
H	2.4395187	0.9516509	-0.2782395
H	1.011835	1.0117973	-1.2655432
H	0.0495185	1.1461004	3.3973972
C	0.11785	0.1497809	3.9872255
H	1.1886033	0.0859035	4.1749108
C	-0.4452477	-1.0073181	3.2184255
H	0.3248905	-1.6646578	2.815414
O	-2.7881914	1.0958721	3.0412647
C	-2.8791331	2.368747	3.6919928
H	-1.8837756	2.6421457	4.0332409
H	-3.5489303	2.2974404	4.5521669
H	-3.2545831	3.1332222	3.0053499
C	-4.0723969	0.6230605	2.6147137
H	-4.4867941	1.2752226	1.8400892
H	-4.7584117	0.5933888	3.4647505
H	-3.9391125	-0.3805179	2.2211088
H	-0.426248	0.3756995	4.9038271
C	-1.566299	-1.8037803	3.8488515
H	-1.1611543	-2.2588247	4.7631919
H	-2.3630451	-1.1357812	4.181346
C	-2.1255054	-2.9153571	2.962531
H	-1.3402549	-3.6109452	2.6569488
H	-2.5912605	-2.5196991	2.0569394
H	-2.8813482	-3.4924216	3.4962493
H			
C	-0.2468902	2.3973674	-0.0615701
H	-0.5509322	3.3642531	0.3311538
C	-1.2506192	1.5874992	-0.4495347
H	-2.2581594	1.9581741	-0.3020648
C	0.1892244	-1.0979333	0.6860015
C	1.2007154	-0.1119206	0.9086879
C	-0.9971852	-0.8224425	0.0041606
H	-1.7769485	-1.5716682	0.0778948
H	0.2409772	-2.0248628	1.2378425
H	1.9466323	-0.4061358	1.6391714
C	-1.1699031	0.2191063	-1.0898361
H	-0.3758157	0.1559032	-1.8336399
H	-2.1017931	0.0247084	-1.6193134
C	1.2401935	2.2300525	-0.2089472
H	1.7233621	2.7966119	0.5922101
H	1.5619297	2.7216368	-1.134595
C	1.7600005	0.7894185	-0.1958339
H	2.8452667	0.823141	-0.0846162
H	1.5818345	0.3202133	-1.1629148
C	-2.1180903	-2.6577112	4.4842287
Rh	-0.6209599	0.521646	1.8153773
H	-1.3723342	-2.9166227	5.2367014
H	-2.6843016	-3.5632115	4.2585023
O	-2.8156247	1.3656587	2.5624155
N	-0.3697508	2.17937	4.3436894
N	-0.9495179	2.1369662	5.2858187

C	0.2537014	2.1078265	3.1241324
H	0.1570435	3.0835619	2.6530311
H	1.2916564	1.833004	3.2983097
C	-3.2005413	2.7152693	2.2974611
H	-2.2980925	3.3001802	2.1381432
H	-3.7543109	3.1230666	3.1478244
H	-3.8298857	2.7764169	1.4045123
C	-3.9691409	0.5378782	2.7574731
H	-4.5578531	0.4798989	1.8370712
H	-4.5906265	0.9459635	3.5591702
H	-3.6266596	-0.4522001	3.0365888
C	-1.4716201	-2.094947	3.2093298
H	-2.2577202	-1.9266608	2.4691853
H	-0.8199966	-2.8641976	2.7858161
C	-0.6772117	-0.8075625	3.4603341
H	-2.8064304	-1.9384799	4.935534
H	-1.2778159	-0.1782201	4.1266833
C	0.6716894	-1.1002307	4.1029304
H	1.235855	-0.2039998	4.366256
H	1.3063858	-1.7107	3.4570684
H	0.5381625	-1.6657089	5.031067

TS5

C	-0.1733469	2.2643904	-0.1789368
H	-0.4787683	3.2503533	0.1587966
C	-1.1759782	1.4155911	-0.5026953
H	-2.1862673	1.7766491	-0.3541927
C	0.2354682	-1.1510336	0.7560068
C	1.2185097	-0.1178456	0.9872014
C	-0.879407	-0.9943776	-0.0357662
H	-1.6305541	-1.7740284	0.0222085
H	0.2663376	-2.032312	1.3816376
H	1.9375398	-0.3699879	1.7583072
C	-1.0596825	0.044951	-1.1302927
H	-0.2506167	-0.00409	-1.8600822
H	-1.9770666	-0.1705289	-1.6769358
C	1.3062878	2.0895753	-0.3941257
H	1.8283043	2.7828896	0.2689082
H	1.560069	2.4227617	-1.4068845
C	1.8426759	0.667249	-0.1761123
H	2.9183264	0.7323729	-0.0050601
H	1.7297252	0.0831702	-1.0895447
C	-2.2624345	-2.187177	4.7138017
Rh	-0.5838127	0.6195352	1.7938289
H	-1.487641	-2.6190207	5.348632
H	-3.0155101	-2.9589342	4.5451996
O	-2.9437928	1.3201476	2.2987245
N	0.3161413	2.2811965	4.4402436
N	0.2921457	1.9572092	5.4857133
C	0.0978238	2.2877904	2.6677756
H	-0.5547772	3.1635971	2.6922521
H	1.122316	2.6053858	2.4770747
C	-3.365154	2.0241552	3.4664194
H	-2.4902364	2.4858593	3.9163443
H	-3.8264934	1.3432212	4.1884468
H	-4.0832024	2.8054523	3.2016864
C	-4.0591921	0.7308044	1.6246806
H	-4.7591555	1.5062437	1.3000329
H	-4.5830692	0.029174	2.2806677
H	-3.6799541	0.1963579	0.7583505

C	-1.6957262	-1.6885624	3.3748715
H	-2.5302729	-1.3389723	2.7628237
H	-1.2569469	-2.5363951	2.8422341
C	-0.6592274	-0.5742233	3.5426355
H	-2.73644	-1.3751536	5.2705254
H	-1.0771183	0.1574407	4.2405438
C	0.6727624	-1.0831713	4.0756935
H	1.4207152	-0.2968981	4.1864794
H	1.1031566	-1.8566577	3.4367432
H	0.5414386	-1.5347776	5.0640498

I

C	-0.3151792	2.3049016	-0.0742555
H	-0.6273018	3.2436386	0.37368
C	-1.3012626	1.470805	-0.4646616
H	-2.3204872	1.7843326	-0.2719026
C	0.0891139	-1.1896767	0.5107712
C	1.0667118	-0.169806	0.8915734
C	-0.9401869	-1.013798	-0.3568426
H	-1.6485012	-1.8292326	-0.4590833
H	0.1255665	-2.1325639	1.0414332
H	1.8017063	-0.5507134	1.5905854
C	-1.1590615	0.1872478	-1.2542309
H	-0.3506539	0.2649978	-1.9840166
H	-2.0719931	0.0343972	-1.8288323
C	1.1636879	2.1526613	-0.3017214
H	1.6811364	2.7936646	0.4149244
H	1.4192163	2.5669225	-1.2840166
C	1.7092719	0.7199928	-0.1889122
H	2.7790312	0.7825401	0.0146517
H	1.6261037	0.2084851	-1.148575
C	-2.2061765	-2.2706393	4.6615477
Rh	-0.5802066	0.6254621	1.8997138
H	-1.4680505	-2.6209972	5.3842101
H	-2.7844986	-1.4730623	5.1319727
O	-2.8754012	1.114176	2.5396276
C	0.3179216	1.8524701	2.9288816
H	0.9622298	2.6298196	2.5115348
H	0.2930266	1.8734011	4.0215093
C	-3.1650996	2.3017266	3.2895747
H	-2.3057056	2.514621	3.9192607
H	-4.0422861	2.1377891	3.9195588
H	-3.3516828	3.1470002	2.6204946
C	-4.0221913	0.6606268	1.8125248
H	-4.3468273	1.412496	1.0866744
H	-4.8427099	0.4521659	2.5033315
H	-3.7493616	-0.255429	1.2944252
C	-1.5441269	-1.7814056	3.3635155
H	-2.3387554	-1.476349	2.6773035
H	-1.0288625	-2.6187641	2.8858897
C	-0.563815	-0.6351738	3.6053263
H	-1.0110835	0.0624397	4.3196778
H	-2.8846632	-3.0999167	4.4541047
C	0.7875292	-1.1036506	4.112854
H	1.4688785	-0.2801708	4.3329335
H	1.2842789	-1.7729762	3.4071554
H	0.6610098	-1.6692259	5.042083

TS6

C	-0.2917459	2.2422235	-0.0061435
---	------------	-----------	------------

H	-0.6529849	3.1578193	0.4501457
C	-1.2455807	1.3758091	-0.45157
H	-2.2792587	1.6420117	-0.2700724
C	0.2209272	-1.1784452	0.5270512
C	1.1547693	-0.1181073	0.9049946
C	-0.8094671	-1.0447816	-0.3538664
H	-1.5097249	-1.8691456	-0.4308092
H	0.2654764	-2.1061864	1.0833078
H	1.866244	-0.4381106	1.6572938
C	-1.028688	0.1326783	-1.2830491
H	-0.1988942	0.2474614	-1.9813065
H	-1.918617	-0.0464615	-1.8846242
C	1.1910532	2.185669	-0.2699459
H	1.6806093	2.8502838	0.4428681
H	1.3934665	2.6111905	-1.2598551
C	1.8019412	0.7801432	-0.1636986
H	2.8632709	0.8815715	0.0653705
H	1.7577749	0.2696857	-1.1262918
C	-2.0115316	-2.34694.7562762	
Rh	-0.5903321	0.6169742	1.7491562
H	-1.2047922	-3.0112936	5.0666965
H	-2.2212483	-1.659954	5.5791409
O	-2.9956935	1.4199376	2.2632608
C	0.0566033	1.6364831	3.1453042
H	1.1129233	1.7842661	3.3803463
H	-0.6017775	2.1041253	3.880771
C	-3.3305939	2.6223727	2.9564519
H	-2.4105383	3.1714949	3.1416696
H	-3.8205557	2.3981105	3.9089241
H	-3.9969589	3.2421908	2.3489468
C	-4.165102	0.6922146	1.8826416
H	-4.8002418	1.3009469	1.2315975
H	-4.742342	0.3943476	2.7635137
H	-3.8434463	-0.1975794	1.3460781
C	-1.6669424	-1.5837521	3.4661275
H	-2.5473769	-1.015483	3.1655897
H	-1.462079	-2.3004287	2.6673753
C	-0.4748081	-0.6412326	3.64129
H	-0.6997411	0.0024999	4.4945545
H	-2.9005555	-2.9604752	4.5998011
C	0.8536877	-1.3294768	3.8971033
H	1.6805274	-0.6257081	3.9964536
H	1.1122784	-2.0551013	3.1254769
H	0.8003546	-1.8786585	4.8419081

J

Rh	-0.7049597	0.4814449	1.7031362
C	0.0915009	2.6329119	0.6646007
H	0.2758709	3.3462392	1.4632948
C	-1.2079552	2.4592503	0.3226025
H	-1.9414979	3.0210891	0.888747
C	-0.8151105	-0.7289567	-0.0365426
C	0.5317805	-0.2908371	0.1361433
C	-1.8747084	0.1791791	-0.1810819
H	-2.8715809	-0.2338336	-0.0742208
H	-1.068306	-1.7587789	0.1864821
H	1.2031743	-1.0688772	0.4850914
C	-1.7823247	1.5775532	-0.7694824
H	-1.1996595	1.603694	-1.6884677
H	-2.7818487	1.9266165	-1.0243161

C	1.3382795	2.1411014	-0.024848
H	2.1369584	2.1017246	0.7193863
H	1.6559052	2.8950365	-0.7546777
C	1.2202273	0.776712	-0.7124874
H	2.2250232	0.4246705	-0.9512939
H	0.7076706	0.8720365	-1.6685138
H	0.4993311	0.7479349	3.1336088
C	0.5049906	-0.318929	3.6516662
C	-0.4831532	-1.1595355	2.9060768
H	-0.0796021	-2.0396414	2.4124316
O	-2.3612902	1.2274188	3.1806662
C	-2.36949	2.54353	3.7443729
H	-1.3411773	2.8927478	3.7904528
H	-2.7872523	2.512512	4.7535824
H	-2.9648056	3.2266553	3.131693
C	-3.6775775	0.6644864	3.1112022
H	-4.3045447	1.2369035	2.4212186
H	-4.1370123	0.6669303	4.10271
H	-3.5803052	-0.3587111	2.7588299
H	-1.4065955	-1.3840504	3.4355805
C	0.0945006	0.0030051	5.102135
H	0.197076	-0.9275499	5.6690827
H	-0.9669946	0.2533554	5.115066
C	0.8984311	1.109746	5.7808705
H	0.5048367	1.3062861	6.7792051
H	0.8499447	2.0474833	5.2193788
C	1.9594074	-0.7832983	3.5253759
H	2.6613066	-0.0187768	3.8563647
H	2.2125213	-1.0508549	2.5005802
H	2.107469	-1.6678308	4.14852
H	1.9503588	0.84607	5.8958944

K

C	-0.1291415	2.3569508	-0.0677085
H	-0.3167866	3.3563199	0.3140906
C	-1.2164328	1.62794	-0.3775476
H	-2.1826239	2.0849002	-0.1990869
C	0.0186139	-1.1466523	0.8107214
C	1.102804	-0.2357175	0.9952125
C	-1.1386929	-0.7949987	0.1239057
H	-1.9702153	-1.4830504	0.2222025
H	-0.0063181	-2.0523237	1.4012764
H	1.8267126	-0.5626243	1.7337927
C	-1.2582204	0.2413135	-0.9835932
H	-0.4878646	0.1019765	-1.7421372
H	-2.2132812	0.10489	-1.4893093
C	1.3210927	2.0338651	-0.2999823
H	1.9171023	2.6449198	0.3803495
H	1.6020811	2.3803784	-1.3012016
C	1.7251043	0.5578564	-0.1594689
H	2.8094968	0.516865	-0.0440007
H	1.5128304	0.0284923	-1.0880304
C	-1.8784541	-2.6675089	4.7236698
Rh	-0.6707147	0.5802878	1.9060759
H	-0.9181165	-3.1901119	4.7752611
H	-1.9402824	-2.0496628	5.6249286
O	-3.0826615	1.1392471	2.3372036
C	-3.5828827	2.4067497	2.7761771
H	-2.854065	2.8511	3.4447062
H	-4.5217677	2.2663636	3.3176385

H	-3.758102	3.0736172	1.9254534
C	-4.0842403	0.4417607	1.5901522
H	-4.312234	0.967505	0.656966
H	-5.0003709	0.3573004	2.1802736
H	-3.7096443	-0.5529568	1.3728662
C	-1.892212	-1.75493	3.4825167
H	-2.8558472	-1.2426217	3.4432696
H	-1.8350217	-2.3907449	2.5930953
C	-0.7628417	-0.741333	3.5185018
H	0.2082717	-1.2338445	3.597257
H	-0.8847961	-0.0900519	4.3839748
C	-3.0185994	-3.6844921	4.7190264
H	-2.9826859	-4.3165884	5.6077014
H	-2.9637778	-4.3390115	3.8456041
H	-3.9928667	-3.1896926	4.7044866
C	0.9614884	1.8559716	3.2099954
H	1.5563425	2.2578062	2.3996952
C	-0.3136772	2.3240249	3.3564897
H	-0.6685389	3.1464674	2.7503169
H	-0.8661076	2.1209836	4.2658355
C	1.7403417	1.1243831	4.2555785
H	2.4229865	1.8435127	4.7215201
H	2.363689	0.3335113	3.8368182
H	1.1125859	0.708685	5.0403834

TS7

C	-0.3135555	2.0818693	0.0097799
H	-0.6112585	3.0041762	0.4955958
C	-1.3237225	1.1909726	-0.2679459
H	-2.3163015	1.4573578	0.0754755
C	0.3048767	-1.3395275	0.260225
C	1.2215544	-0.2325152	0.5610444
C	-0.8226053	-1.2365355	-0.4834229
H	-1.4477365	-2.1176718	-0.578507
H	0.4916221	-2.2948994	0.7395464
H	2.0288509	-0.5317984	1.2259744
C	-1.2690593	0.010375	-1.2140655
H	-0.6185475	0.2062064	-2.0711424
H	-2.2660533	-0.1532585	-1.6219833
C	1.0829724	2.0727936	-0.5613859
H	1.6962108	2.7435192	0.0422446
H	1.0736662	2.5074949	-1.5670893
C	1.7143382	0.6745997	-0.5815356
H	2.7987556	0.7683757	-0.5157092
H	1.5169197	0.1776786	-1.5321632
C	-1.4800584	-2.776664	4.3696273
Rh	-0.3508828	0.5103917	1.657911
H	-0.8864651	-3.508463	3.8131166
H	-0.9936371	-2.6653843	5.3435662
O	-3.0520357	1.5114028	2.5476689
C	-3.3975858	2.8338485	2.9450278
H	-2.4765743	3.4029019	3.0582754
H	-3.9334735	2.8284366	3.9001335
H	-4.0263714	3.3191174	2.1907533
C	-4.2098648	0.7003631	2.375831
H	-4.8758956	1.1248159	1.6163519
H	-4.7650305	0.6046777	3.314988
H	-3.8811151	-0.2854163	2.0544792
C	-1.4413148	-1.4219416	3.634854
H	-2.017799	-0.6924529	4.2092402

H	-1.9514756	-1.5329507	2.6730771
C	-0.0132414	-0.9380268	3.4460146
H	0.5728133	-1.5506805	2.7649862
H	0.5123721	-0.9992958	4.3903685
C	-2.9010403	-3.30415	4.559825
H	-2.894197	-4.2567508	5.091541
H	-3.3981939	-3.4658642	3.6002109
H	-3.5098323	-2.6061456	5.139469
C	0.5979978	1.0685041	3.8479683
H	1.6157303	0.7143739	3.9624834
C	0.4109398	2.0395448	2.8108619
H	1.3034441	2.4340972	2.3364484
H	-0.3537314	2.7919023	2.9840382
C	-0.1643522	1.2549723	5.1340473
H	0.2350813	2.1438246	5.6314759
H	-0.0591692	0.4173985	5.8219591
H	-1.2245105	1.431428	4.9513883
L			
Rh	-0.6703254	0.4692012	1.5913992
C	-0.0096195	2.6585878	0.531142
H	0.2494222	3.3534798	1.3253528
C	-1.3355561	2.4754744	0.3223392
H	-2.0118924	3.0119722	0.9772334
C	-0.948442	-0.6971198	-0.1598424
C	0.4044019	-0.2461147	-0.1166002
C	-2.02722	0.1996293	-0.1687809
H	-3.0028227	-0.2299646	0.0294907
H	-1.1655945	-1.7356475	0.0607559
H	1.1165084	-1.0239149	0.1386087
C	-2.0123097	1.6135387	-0.726021
H	-1.5304148	1.6704367	-1.7003704
H	-3.0368664	1.9557901	-0.8647402
C	1.1632478	2.2009739	-0.2973719
H	2.0360671	2.1544733	0.3576883
H	1.3941101	2.9764409	-1.0370446
C	0.9883448	0.8522185	-1.0036623
H	1.9661939	0.5201287	-1.355944
H	0.3771846	0.9645394	-1.8980006
H	0.6718208	0.7116968	2.895331
C	0.7418528	-0.3686136	3.3830764
C	-0.312079	-1.1994834	2.7220926
H	0.0430478	-2.0625429	2.1652659
O	-2.1662853	1.1637573	3.2497966
C	-2.1033558	2.45634	3.8618823
H	-1.0695726	2.7907786	3.828222
H	-2.4284009	2.3897972	4.9028631
H	-2.7413208	3.1702479	3.3328238
C	-3.487576	0.6107717	3.2924273
H	-4.1764769	1.2129472	2.692765
H	-3.8436267	0.5755675	4.3249502
H	-3.435105	-0.398015	2.8922816
H	-1.1749757	-1.4447404	3.3372776
C	0.4778321	-0.0826722	4.875547
H	0.6383053	-1.0265541	5.4047081
H	-0.5821086	0.1446473	4.988622
C	1.3340182	1.0337732	5.5094471
H	0.6956811	1.6429805	6.1559288
H	1.6874184	1.7113221	4.7233121
C	2.5339686	0.5613416	6.3450453

H	3.1591685	1.4299904	6.5697734
H	3.1598157	-0.1146556	5.7552989
C	2.1419134	-0.1175969	7.6575469
H	3.0271241	-0.4180522	8.2204551
H	1.5421141	-1.0165726	7.4955522
H	1.561033	0.557964	8.2905298
C	2.1780125	-0.8106182	3.0864079
H	2.9036106	-0.0513024	3.3757825
H	2.3241788	-1.0311021	2.0300198
H	2.3983341	-1.7185137	3.6515955

Propene

C	-0.1848835	0	1.3785015
H	-1.2697007	0	1.3974341
H	0.3196452	0	2.3367759
C	0.4906585	0	0.2358343
H	1.577703	0	0.2713666
C	-0.119797	0	-1.1309543
H	0.1982024	0.8772942	-1.7029425
H	-1.2100264	0	-1.0830746
H	0.1982024	-0.8772942	-1.7029425

M

Rh	-0.2099242	0.0692433	-0.1694002
C	-0.5053247	-1.3649775	1.3922041
H	-0.8917244	-2.2621965	0.9185858
C	-1.4091574	-0.301985	1.5487824
H	-2.4258498	-0.4678774	1.2035732
C	-1.2713784	0.8419395	2.5274476
H	-1.6108868	0.5360251	3.5267794
H	-1.956806	1.630834	2.2068782
C	0.1579375	1.424975	2.616382
H	0.7331153	0.8936011	3.3764595
H	0.0937812	2.4596029	2.9613405
C	0.9008286	1.3890305	1.2937822
H	0.9999767	2.3421944	0.7838404
C	1.7317258	0.3628893	0.8834092
H	2.4526861	0.5888842	0.10189
C	2.0050009	-0.9170527	1.6413626
H	2.4676155	-1.6188785	0.9427884
H	2.7469034	-0.7478251	2.4334207
C	0.7408704	-1.5736066	2.2414021
H	0.9215685	-2.6455457	2.348306
H	0.5648393	-1.1996423	3.2519555
C	-1.4954293	-0.5768947	-1.6472875
H	-2.5239628	-0.2383543	-1.5334634
C	-0.63364	0.2676876	-2.5256673
H	-1.1520421	1.1496577	-2.9102346
C	0.1514418	-0.4311947	-3.6392712
H	-0.5702102	-0.7998191	-4.3750509
C	1.1784617	0.4639417	-4.3292077
H	0.7028032	1.3396948	-4.7786575
H	1.7013202	-0.0726105	-5.1236432
H	1.9308431	0.8227384	-3.621427
H	-1.4516793	-1.6477405	-1.8474679
H	0.6448049	-1.3140245	-3.2233363
H	0.2024911	0.7882863	-1.8664754

N

Rh	-0.2742739	-0.093015	-0.1326433
C	0.5563029	1.8599662	-0.3381043
H	0.6382459	2.2877454	0.6561623
C	-0.7229027	1.852512	-0.9173537
H	-1.5288236	2.2529945	-0.3111994
C	-0.9945181	1.8470719	-2.415661
H	-0.2007513	2.3850581	-2.9381589
H	-1.9109726	2.4084165	-2.6117881
C	-1.150712	0.4271652	-2.9992862
H	-0.9554264	0.442399	-4.0804441
H	-2.1921366	0.1143713	-2.8880497
C	-0.2902091	-0.6117724	-2.3159523
H	-0.6768051	-1.6255012	-2.3909298
C	1.032792	-0.462327	-1.9449822
H	1.5898882	-1.3673108	-1.7176294
C	1.8817159	0.763379	-2.2325165
H	2.9113062	0.4466702	-2.4152162
H	1.5469528	1.2324081	-3.1591761
C	1.871157	1.7919529	-1.081754
H	2.6429302	1.5208642	-0.3566403
H	2.1525219	2.7836297	-1.46312
C	-0.9212178	0.4512048	1.8002499
C	-0.621946	-2.1549376	0.6259806
H	-1.7868472	-0.1714681	2.0713157
C	0.1425822	0.3352559	2.8962082
H	0.5424794	-0.6867492	2.9468367
C	-0.3529076	0.7208807	4.298197
H	-1.2075213	0.0874166	4.562171
C	0.7223898	0.6087171	5.3791515
H	1.1013784	-0.4144819	5.4565849
H	0.3374704	0.8934932	6.3615296
H	1.5744589	1.2573237	5.1567914
H	-0.3581141	-2.2138832	1.6771645
N	0.0652773	-3.0788323	-0.0780149
N	0.6805775	-3.7535	-0.7196102
H	-1.6865392	-2.2207923	0.4027907
H	-1.2936153	1.4822652	1.7813549
H	1.0047548	0.9661692	2.6489252
H	-0.7369421	1.7462405	4.2678166

N'

Rh	-0.178914	-0.1831859	-0.0439825
C	0.3942746	1.8577259	-0.4009319
H	0.5086466	2.3176513	0.5754215
C	-0.9146871	1.6730982	-0.8627664
H	-1.709702	1.9952618	-0.1993714
C	-1.3154884	1.5698072	-2.328856
H	-0.6466261	2.1782823	-2.940237
H	-2.3090503	2.0066609	-2.4530949
C	-1.3472431	0.1185201	-2.8496015
H	-1.2656107	0.1090942	-3.9449193
H	-2.3219288	-0.3172773	-2.6176211
C	-0.29587	-0.7744618	-2.2337543
H	-0.560614	-1.8273161	-2.2024494
C	1.0225474	-0.4478232	-2.004404
H	1.7015403	-1.2588865	-1.765583
C	1.6755417	0.8654628	-2.3847534
H	2.7151561	0.6766551	-2.6628117
H	1.1973236	1.2694826	-3.2777977
C	1.6462105	1.9062316	-1.2458856

H	2.49621	1.7287581	-0.5822098
H	1.7903339	2.9148901	-1.6578351
C	-0.8375557	0.3832218	1.8759175
H	-1.7017334	-0.2556041	2.0998696
C	0.2018421	0.2602698	2.9903025
H	0.566605	-0.7712019	3.0556499
C	-0.3186688	0.6843389	4.3714808
H	-1.1977909	0.0798333	4.6223587
C	0.725408	0.5548657	5.4805213
H	1.0714248	-0.4779776	5.5784175
H	0.3246014	0.8633559	6.4492717
H	1.6018145	1.1750013	5.2720459
H	-1.2117707	1.4115055	1.8398649
H	1.0838245	0.8667653	2.7507577
H	-0.6706918	1.7202976	4.3187451
N	0.043704	-2.023171	0.6341585
N	-0.2737366	-3.1025348	0.8632829
C	-0.5986682	-4.3124866	1.1410419
H	-0.9941839	-4.5283968	2.1221031
H	-0.4708901	-5.0706475	0.3832288

TS8

Rh	0.3952519	0.4526811	0.1778607
C	-1.4414092	-0.803544	0.0802936
H	-1.6377931	-0.9485579	-0.9750634
C	-1.7863189	0.4298154	0.6199482
H	-2.209137	1.1566017	-0.0644354
C	-2.0762772	0.6934786	2.0924191
H	-2.5531471	-0.1820357	2.5353624
H	-2.8127811	1.4971649	2.1629817
C	-0.8377715	1.1027749	2.9157628
H	-1.0403172	0.9660635	3.9865675
H	-0.6651093	2.173053	2.7812655
C	0.4422498	0.3887783	2.5468591
H	1.3472143	0.9525174	2.7417015
C	0.5807162	-0.9254644	2.2157516
H	1.5915871	-1.3107388	2.1330053
C	-0.5263869	-1.9564285	2.2008272
H	-0.1029124	-2.9259203	2.4732892
H	-1.2524017	-1.7198576	2.9786234
C	-1.2354387	-2.0979453	0.8375646
H	-0.6453598	-2.7620207	0.2018932
H	-2.2004603	-2.6031081	0.9807115
C	0.0910081	1.5015682	-1.62315
C	2.3460861	0.9396895	0.0487149
H	1.0651793	1.6807978	-2.0873974
C	-0.8733724	0.9939502	-2.6939775
H	-1.8610495	0.7776243	-2.2706783
C	-0.3831788	-0.2234098	-3.4804948
H	-0.2220932	-1.065274	-2.8006197
C	-1.338199	-0.6468492	-4.5962883
H	-2.3222688	-0.9091678	-4.1971763
H	-0.9593838	-1.5161944	-5.1387573
H	-1.4838504	0.1592234	-5.3208699
H	2.8097802	1.2937691	-0.8705566
N	1.8688987	-0.7433896	-0.6447877
N	2.1538702	-1.7223144	-1.1058431
H	3.0775362	0.6031315	0.7848377
H	-0.2546002	2.4699494	-1.2427107
H	-1.0475145	1.8088539	-3.4124563

H	0.5991539	0.0047344	-3.9089779
---	-----------	-----------	------------

O

Rh	0.6309138	0.1005086	0.00822
C	-1.5495959	0.7523025	0.9297498
H	-1.6342057	-0.0161398	1.688807
C	-1.7183159	0.3730292	-0.3665908
H	-1.9685163	-0.6645905	-0.5540776
C	-1.8128895	1.27319	-1.5725806
H	-2.8453099	1.6243056	-1.7017422
H	-1.5900388	0.6655354	-2.4521722
C	-0.848794	2.4763877	-1.5454833
H	-1.3004613	3.31326	-1.0108999
H	-0.7049675	2.8247694	-2.5706816
C	0.5106427	2.1575891	-0.9489343
H	1.3267552	2.146537	-1.661797
C	0.8645244	2.2795927	0.3910175
H	1.9221896	2.3912751	0.6070853
C	-0.0303469	2.7009613	1.5305682
H	0.4234444	2.3362232	2.4552891
H	-0.0401131	3.7966291	1.6111042
C	-1.4750253	2.1724887	1.4402013
H	-1.9236323	2.2111001	2.4356246
H	-2.0801465	2.8275976	0.8139806
C	0.19075	-1.9050964	0.620649
H	-0.8507536	-1.9020303	0.9488382
C	2.3894984	-0.2713589	-0.3392592
H	3.217771	-0.1281103	0.3641189
C	0.4155451	-3.002506	-0.4214145
C	-0.0136563	-4.411635	0.0291334
H	0.4780457	-4.6460561	0.9802288
H	-0.110902	-2.7624875	-1.3534104
C	-1.5239205	-4.6005742	0.1758781
H	-1.9440275	-3.9402438	0.937565
H	-1.7694496	-5.6262133	0.4615581
H	-2.0378071	-4.3887327	-0.7666803
H	2.746052	-0.5704574	-1.3317211
H	0.8011202	-2.1043241	1.5060741
H	1.4774266	-3.0320215	-0.6839303
H	0.3631962	-5.1407045	-0.6973162

TS9

Rh	0.651104	0.245577	0.0786097
C	-1.4807728	0.7101544	0.8949079
H	-1.5906534	-0.046702	1.6634435
C	-1.5853333	0.2963677	-0.4098375
H	-1.8102979	-0.7509207	-0.5792393
C	-1.7224855	1.1774147	-1.6283462
H	-2.772824	1.4619925	-1.7778392
H	-1.4473629	0.5766629	-2.4983723
C	-0.8339068	2.4389414	-1.5948164
H	-1.3531341	3.2558319	-1.0910707
H	-0.6723151	2.7779585	-2.620529
C	0.5166247	2.2028373	-0.9382894
H	1.3621858	2.19492	-1.6166456
C	0.8005364	2.4015144	0.4114916
H	1.841323	2.5595829	0.675186
C	-0.1743153	2.8212934	1.4841142
H	0.2707692	2.5621509	2.4479756
H	-0.29088	3.9136368	1.4884649

C	-1.5568395	2.1455883	1.3748769
H	-2.0346678	2.1628348	2.356932
H	-2.2082708	2.7204531	0.7156574
C	0.5202241	-1.9458813	0.5763225
H	-0.3440251	-1.8881254	1.2408168
C	2.3302182	-0.5429527	0.0787117
H	2.9609494	-0.6495535	0.9664533
C	0.2592704	-2.835853	-0.6367361
C	-0.0949485	-4.2937813	-0.2892715
H	0.6993388	-4.7139981	0.3381865
H	-0.545202	-2.4230459	-1.2551121
C	-1.4433503	-4.4670122	0.410454
H	-1.467653	-3.9561956	1.3748389
H	-1.6621857	-5.5220379	0.5920058
H	-2.2562879	-4.0619523	-0.1999256
H	2.7429006	-1.1139891	-0.7588681
H	1.3278198	-2.3769698	1.1738861
H	1.1467037	-2.8456099	-1.2775411
H	-0.0972561	-4.8811323	-1.213895

P

Rh	-0.2554612	0.0927746	-0.1570449
C	-0.4856694	-1.3743839	1.385564
H	-0.8637918	-2.2709207	0.9040726
C	-1.4073181	-0.3339775	1.5820627
H	-2.428051	-0.5151526	1.2566655
C	-1.270995	0.7948916	2.5782974
H	-1.58131	0.4639734	3.5792122
H	-1.9796301	1.5747276	2.2875057
C	0.1475569	1.4063322	2.6456189
H	0.7516017	0.8727694	3.3813802
H	0.0702713	2.4325708	3.0122844
C	0.8589388	1.4113453	1.3052794
H	0.9250583	2.3758031	0.8113912
C	1.7016803	0.4113281	0.8559266
H	2.3996029	0.6673363	0.0626951
C	2.0199208	-0.8759575	1.5832089
H	2.4803158	-1.5547087	0.8607914
H	2.7768562	-0.7049876	2.3605202
C	0.78482	-1.5707353	2.2008584
H	0.9912192	-2.640174	2.2837527
H	0.6248457	-1.2187321	3.2218519
C	-1.5514644	-0.5658037	-1.621151
H	-2.5815952	-0.2381528	-1.4903461
C	-0.7091421	0.2939553	-2.5036983
H	-1.2477843	1.1657755	-2.8789529
C	0.0839356	-0.4018765	-3.6149359
H	-0.6289681	-0.7307815	-4.3793441
C	1.1781298	0.4468601	-4.2709373
H	1.7448351	-0.1898103	-4.9571906
H	1.8902889	0.7701161	-3.5028905
H	-1.498988	-1.6350022	-1.8270822
H	0.5320225	-1.3092134	-3.2003825
H	0.123151	0.8290346	-1.8474726
C	0.6628798	1.6674316	-5.0356931
H	1.4829033	2.2001293	-5.522198
H	0.1582665	2.3785369	-4.37812
H	-0.048208	1.3730186	-5.8127383

TS10

Rh	-0.2063123	0.1130585	-0.2380455
C	-0.5723685	-1.3770058	1.3963094
H	-0.9738366	-2.2390566	0.8743536
C	-1.4217568	-0.2971157	1.5683828
H	-2.4361331	-0.4008878	1.1963022
C	-1.221266	0.8540618	2.525443
H	-1.5593013	0.576906	3.5334191
H	-1.8772891	1.6661146	2.2019454
C	0.2297896	1.3796958	2.5848157
H	0.8004333	0.8285187	3.3343218
H	0.210676	2.4160372	2.9298928
C	0.9442984	1.3199435	1.2455995
H	1.0979554	2.2768572	0.7594498
C	1.7273544	0.2602071	0.8086344
H	2.4607711	0.4717147	0.0369666
C	1.9593454	-1.0395214	1.5431373
H	2.348561	-1.7595174	0.8186689
H	2.7460481	-0.9184095	2.3004388
C	0.691094	-1.6297003	2.198521
H	0.8267383	-2.7075741	2.313458
H	0.5702101	-1.2355675	3.2086559
C	-1.6343724	-0.582535	-1.6520284
H	-2.6156202	-0.1824307	-1.4170152
C	-0.7463886	0.2048053	-2.4327399
H	-1.1091338	1.1867355	-2.7275163
C	0.1650908	-0.4294311	-3.4697564
H	-0.4677941	-0.6798302	-4.3302431
C	1.3202011	0.4492741	-3.9427921
H	0.9565291	1.4031989	-4.3341683
H	1.8838385	-0.0418696	-4.7387417
H	2.0106327	0.6671819	-3.1252638
H	-1.5969589	-1.6639559	-1.7503653
H	0.5464874	-1.3776534	-3.0839344
H	0.3964769	0.9057512	-1.5181055

Q

C	-0.3328449	-1.3866295	1.5349678
H	-0.1728358	-2.3949388	1.1708829
C	-1.4520168	-0.7254569	1.0851057
H	-2.1162259	-1.2689347	0.4227456
C	-2.0450115	0.5377694	1.6599957
H	-2.6782375	0.2995198	2.5254877
H	-2.7153381	0.9569954	0.9056743
C	-1.0024729	1.6055426	2.046754
H	-0.6625799	1.4507977	3.0725914
H	-1.4876368	2.5840931	2.0403506
C	0.1903701	1.6427568	1.1063367
H	0.242518	2.517066	0.4679403
C	1.3765208	0.9328608	1.2882783
H	2.2645217	1.3268745	0.8054068
C	1.6700802	-0.0529721	2.3940926
H	2.5178789	-0.662153	2.0705156
H	2.0067648	0.4754449	3.2970829
C	0.4909381	-0.9859997	2.7420369
H	0.886961	-1.8883976	3.2130816
H	-0.1529473	-0.5186695	3.4888005
C	-0.242613	-1.7390163	-1.6211962
H	-1.3142136	-1.9052144	-1.6171506
C	0.304942	-0.7731961	-2.446463
C	-0.5188071	0.0401401	-3.4193336

H	-1.5248258	0.1857314	-3.0173116
C	0.0806116	1.3815043	-3.8369129
H	0.1387358	2.0668468	-2.9906325
H	-0.5233129	1.8471539	-4.6191237
H	1.0926744	1.2547777	-4.230407
H	1.3560809	-0.8577422	-2.7006319
H	-0.6387739	-0.5796079	-4.3190049
H	0.3631546	-2.5674497	-1.2719596
Rh	0.2559984	-0.0674716	-0.2805229
H	1.0889424	0.8929747	-1.2184773

R

C	-0.3187096	-1.4033092	1.53006
H	-0.1380831	-2.4056921	1.1509586
C	-1.4497772	-0.7503799	1.0879762
H	-2.1041156	-1.2935356	0.4083908
C	-2.0532241	0.4989666	1.6941187
H	-2.6258726	0.2516046	2.5976686
H	-2.7785908	0.8907012	0.9773618
C	-1.0243776	1.607638	2.0145004
H	-0.6562107	1.4987525	3.0374323
H	-1.5334408	2.57301	1.9824892
C	0.1540874	1.6341939	1.0468585
H	0.2307708	2.5383685	0.4515984
C	1.3673049	0.9100556	1.2487046
H	2.2620569	1.3323712	0.8010828
C	1.6541319	-0.0256292	2.4014324
H	2.5348838	-0.6133753	2.1302164
H	1.9377726	0.5448332	3.2970432
C	0.4914513	-0.9887882	2.742187
H	0.9029612	-1.8805041	3.2195744
H	-0.1687294	-0.5320615	3.4817477
Rh	0.2249671	-0.0235274	-0.2051602
H	1.0337436	0.8393072	-1.277242

Alkene

C	-0.1932845	-0.021113	1.3937384
H	-1.2782677	-0.015417	1.4050377
H	0.3037783	-0.0377941	2.3559147
C	0.4895945	-0.0113137	0.2552491
H	1.5775158	-0.0149251	0.2959122
C	-0.1089913	0.0186016	-1.119231
H	-1.199472	-0.0121223	-1.0439316
H	0.1934343	-0.8863102	-1.6599181
C	0.3260089	1.2446875	-1.9320768
H	1.4137257	1.2875658	-2.0289431
H	-0.0012067	2.1687826	-1.4509318
H	-0.0972119	1.2170962	-2.9383128