

**Olefin hydrosilylation catalyzed by
a *bis*-N-heterocyclic carbene rhodium complex.
A density functional theory study**

Yin Wu,¹ Virve A. Karttunen,^{1†} Shane Parker,^{1‡} Alexander Genest,^{1,2} Notker Rösch^{1,2}*

¹ Catalysis Research Center and Wacker-Institut für Siliciumchemie, Technische Universität München, 85747 Garching, Germany

² Institute of High Performance Computing, Agency of Science, Technology and Research, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632, Singapore

Content

S1. Crucial geometry parameters in all optimized structures.....	2
S2. Enthalpy profiles of four most favored pathways.....	4
S3. Pathways of product elimination.....	5
S4. Energetic comparison of the four most favored pathways.....	7
S5. How the conformational changes contribute to receiving lower barriers	7
S6. Enthalpy and entropy contributions as well as solvation terms on crucial barriers	8
S7. Optimized structures for selected intermediates and transition states	8
S8. Zero-point corrected energies, enthalpies and absolute Gibbs free energies	18
S9. Complete Reference 47	20
S10. Geometries	21

* Corresponding author. Email: roesch@mytum.de

† Present address: Department of Chemistry, University of Jyväskylä, P.O. Box 35, Jyväskylä FI-40014, Finland

‡ Present address: Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208-3113, U.S.A.

S1. Crucial geometry parameters in all optimized structures

Table S1. Crucial distances indicating the formation of silylene complex and the product, as well as γ in all optimized structures in the **GT** mechanism.^[a]

	Rh-Si ^[b]		C-Si	C-H	γ
GT1	2.31	-	-	-	106.5
GT2	2.31	-	3.47	3.09	107.8
GT2-3	2.19	-	2.06	1.70	106.8
GT3	2.32	-	1.88	1.09	108.1
GT3-4	2.47	-	1.88	1.10	103.6
GT4	2.41	2.82	1.88	1.09	98.6
GT4-5	2.45	2.75	1.88	1.09	96.4
GT5	2.46	2.67	1.90	1.09	99.0
GT5-6	2.68	2.50	1.89	1.09	96.5
GT6	2.52	2.48	1.89	1.09	99.2
GT6-1	3.02	2.28	1.89	1.09	101.1

[a] Distances are given in Å and angles are given in degrees.

[b] In case of Rh-Si distances, values in first and second columns are given for the first and second silane respectively.

Table S2. Crucial distances indicating the oxidative addition and product formation, as well as γ in all optimized structures in the **CH**, **mCH** and **SBM** mechanism.^[a]

	Si-H ^[b]		C-Si	C-H	γ
CH1	1.70	1.50	3.29	2.60	97.8
CH1-2	1.51	1.52	3.57	2.86	92.0
CH2	1.48	1.60	3.23	2.74	92.2
CH2-3	1.50	2.14	3.18	2.43	89.3
CH3	1.49	2.63	3.18	2.28	107.4
CH3-4	-	-	3.49	1.41	146.8
CH4	-	-	3.39	1.17	150.6
CH4-5	-	-	2.80	1.16	134.7
CH5	-	-	2.63	1.15	102.3
CH5-6	-	-	2.03	1.12	105.3
CH6	-	-	1.90	1.12	101.6
CH6-7	-	-	1.90	1.10	108.8
CH7	-	-	1.90	1.10	108.8

	Si-H ^[b]		C-Si	C-H	γ
CH7-GT3	-		1.90	1.10	100.9
GT4-CH1	-		1.90	1.10	102.4
CH1-2a	4.03	1.49	2.91	2.30	150.1
CH2a	4.12	1.50	3.15	2.41	150.3
CH2a-3a	-		3.35	2.18	142.7
CH3a	-		3.59	2.13	142.0
CH3a-4	-		3.52	1.66	146.8
CH1-2b	2.33	1.50	3.78	1.44	94.9
CH2b	3.09	1.49	2.87	1.16	134.8
CH2b-6	-		2.04	1.13	108.2
CH2-mCH3	2.88	1.48	2.09	2.43	99.8
mCH3	3.14	1.56	1.90	2.43	115.7
mCH3-CH6	-		1.88	1.77	105.2
CH3-3a	-		3.50	2.15	140.6
CH3a-mCHa	-		2.10	2.75	111.1
mCH4a	-		1.90	2.44	127.2
mCH4a-CH6	-		1.89	2.12	109.2
CH3a-mCH4b	-		2.11	2.74	106.5
mCH4b	-		1.90	2.45	132.9
mCH4b-5b	-		1.89	2.32	119.9
mCH5b	-		1.88	2.50	107.2
mCH5b-CH6	-		1.89	1.76	104.1
CH4-SBM5	-		3.77	1.13	153.6
SBM5	-		2.72	1.13	152.7
SBM5-6	-		2.09	1.11	152.7
SBM6	-		1.90	1.10	151.8
SBM6-CH1	-		1.88	1.09	155.6

[a] Distances are given in Å and angles are given in °.

[b] Two Si-H distances are given to demonstrate the isomerization of silane during the oxidative addition.

S2. Enthalpy profiles of four most favored pathways

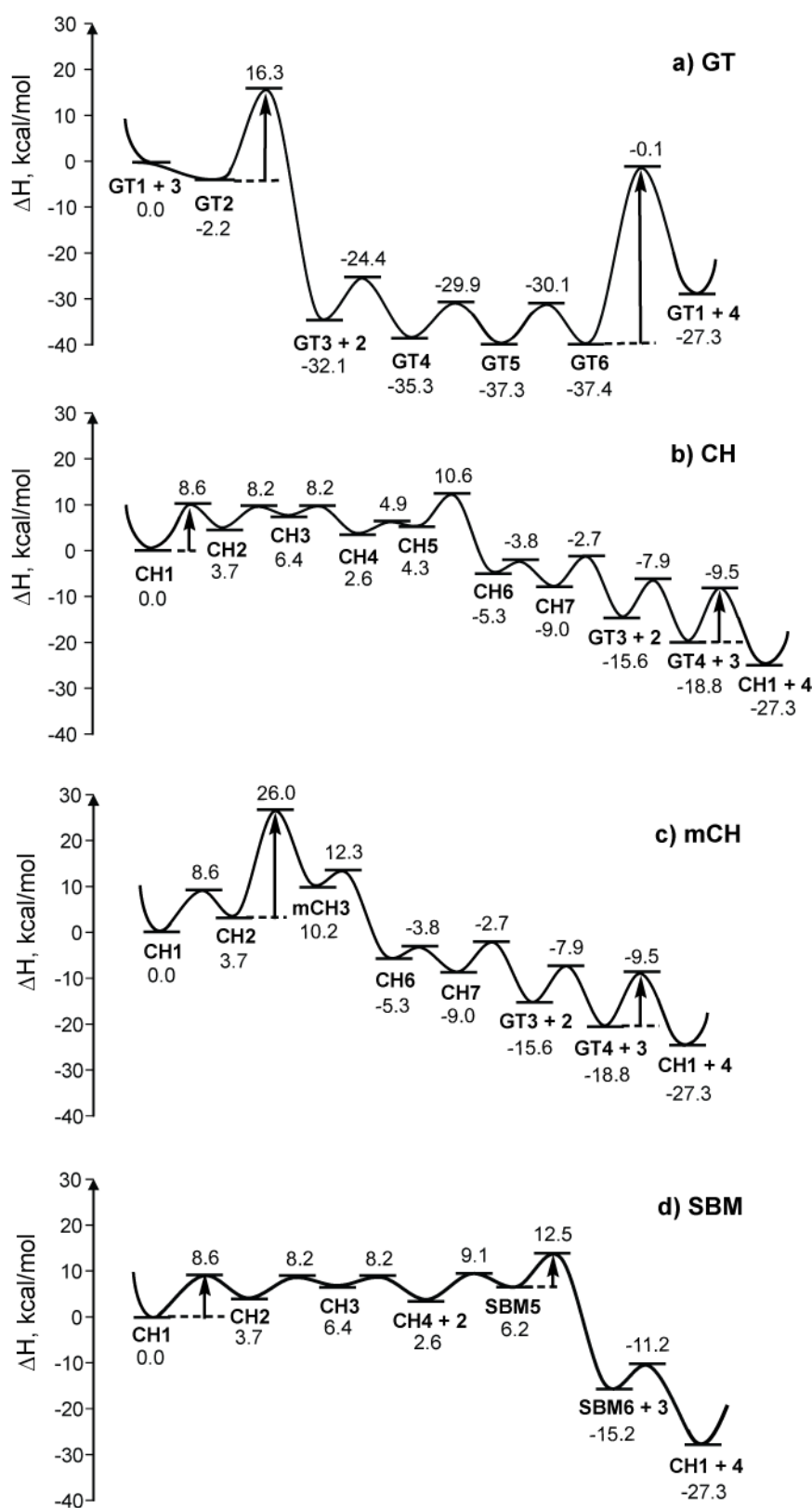
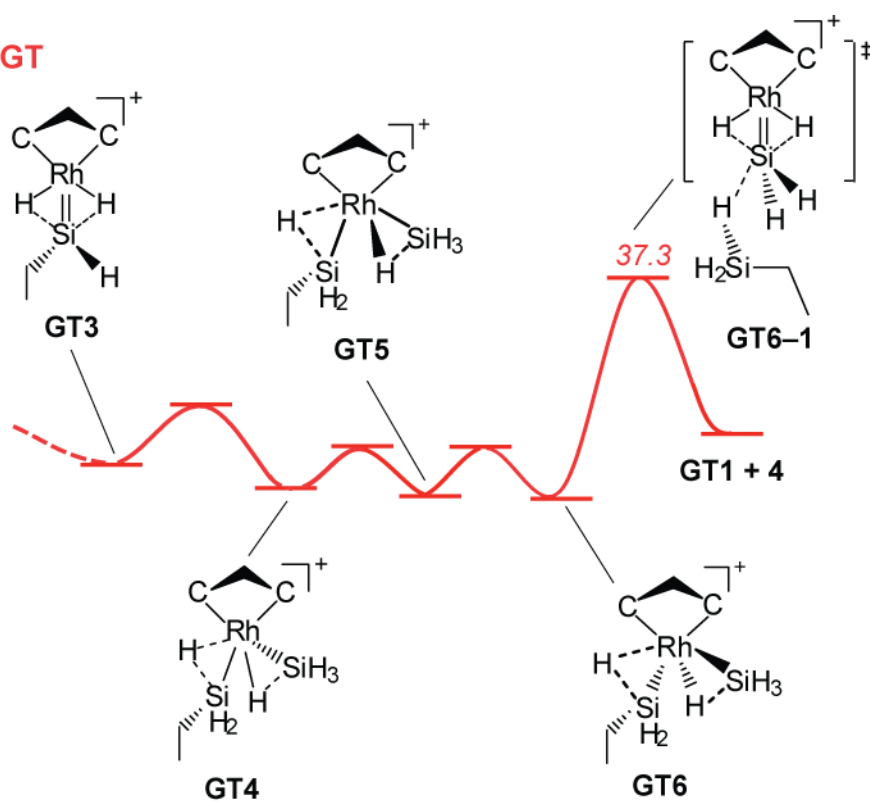


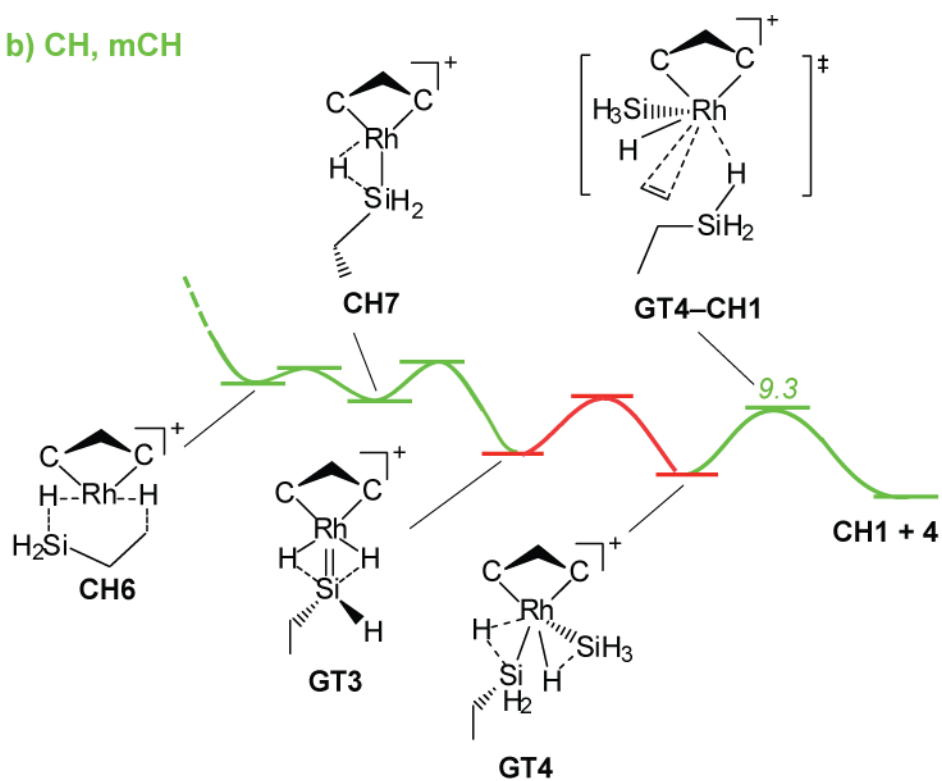
Figure S1. Enthalpy profiles of the most favored pathways in a) **GT**, b) **CH**, c) **mCH** and d) **SBM** mechanisms. Catalytic active species GT1 and CH1 are used as enthalpy references. Comparison of absolute enthalpies of **GT** with **CH**, **mCH** and **SBM** see Figure S5. Crucial steps of each pathway, with highest relative activation barriers, are marked by arrows.

S3. Pathways of product elimination

a) GT



b) CH, mCH



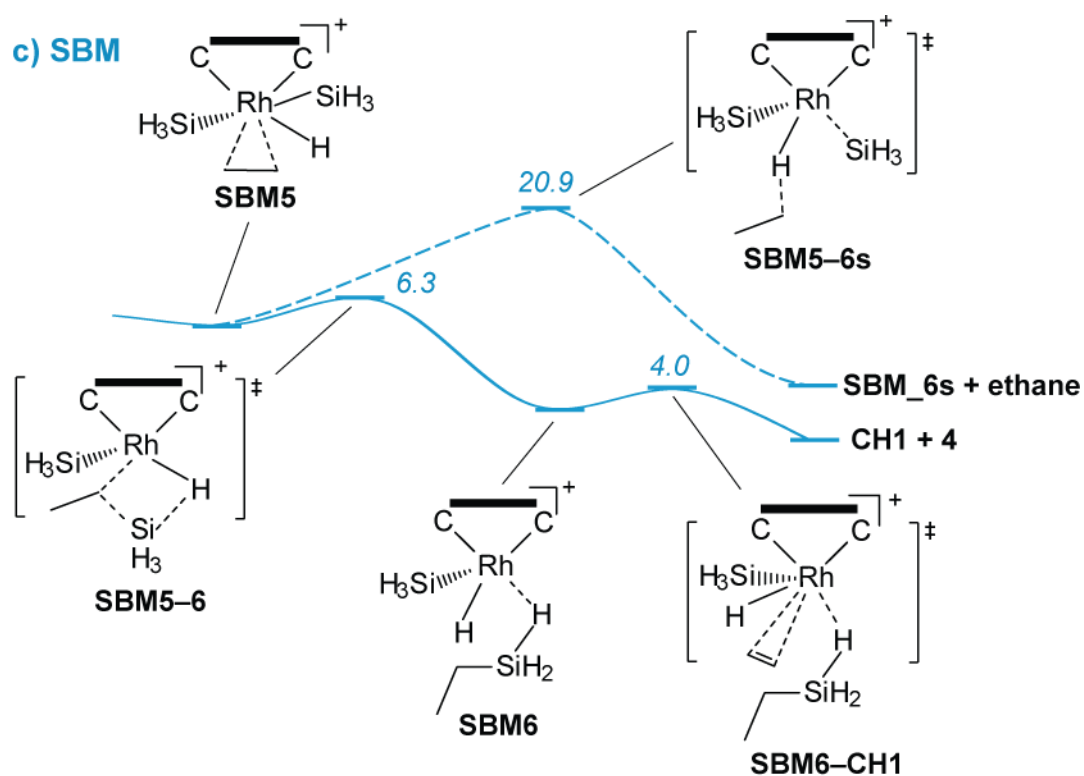


Figure S2. Product elimination for various mechanisms: a) **GT**, b) **CH** and **mCH**, and c) main and side pathways of **SBM**. Relative activation enthalpies $\Delta H^\ddagger$ (kcal·mol⁻¹) of crucial steps.

S4. Energetic comparison of the four most favored pathways

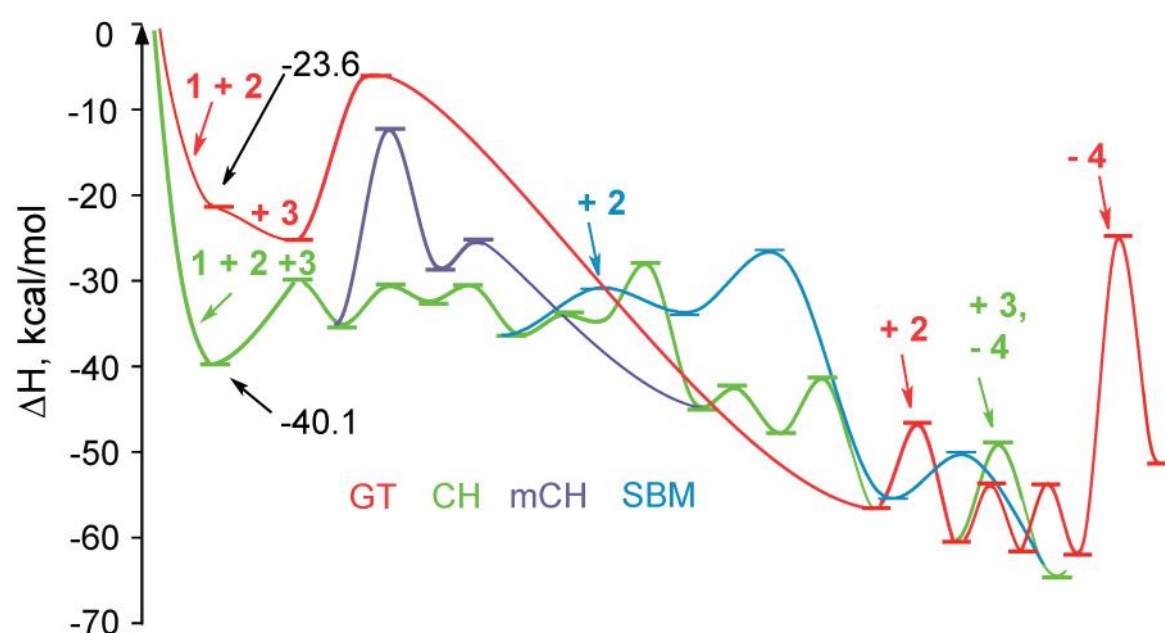


Figure S3. Profiles of the most favored pathways of the mechanisms **GT**, **CH**, **mCH**, and **SBM**, relative to the bare catalyst and separate substrates. Reaction enthalpies for the formation of the catalytically active species **GT1** and **CH1** given in $\text{kcal}\cdot\text{mol}^{-1}$. Steps where reactants are added or the product is eliminated are marked by arrows.

S5. How the conformational changes contribute to receiving lower barriers

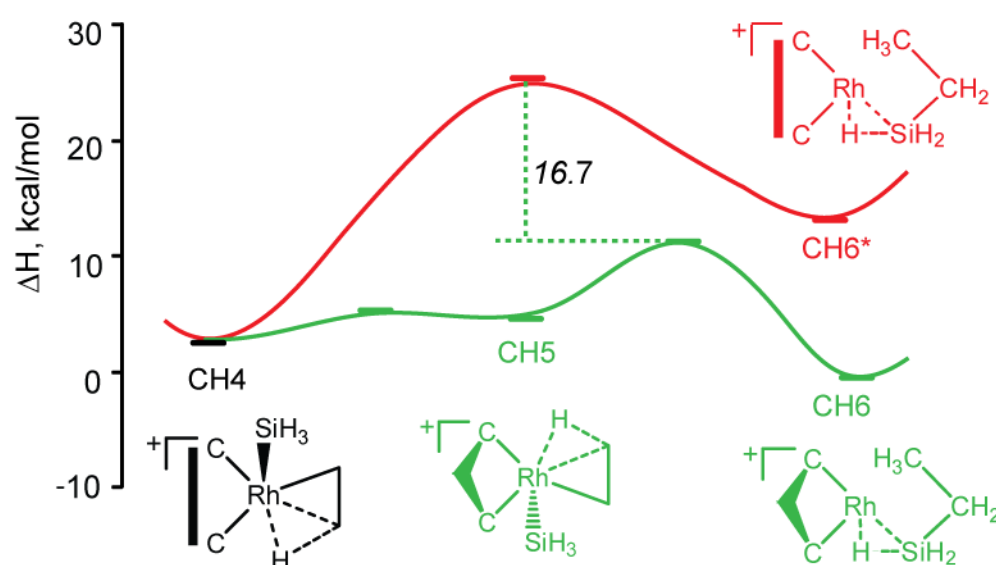


Figure S4. Enthalpy profile **CH4** → **CH5** → **CH6** explored with a flexible *bis*-NHC ligand (green) and with the *bis*-NHC dihedral angle γ fixed at its value for **CH4**, 150° (red). This alternative pathway **CH4** → **CH6** has an activation barrier relative to **CH5** → **CH6** that is by $16.7 \text{ kcal}\cdot\text{mol}^{-1}$ higher.

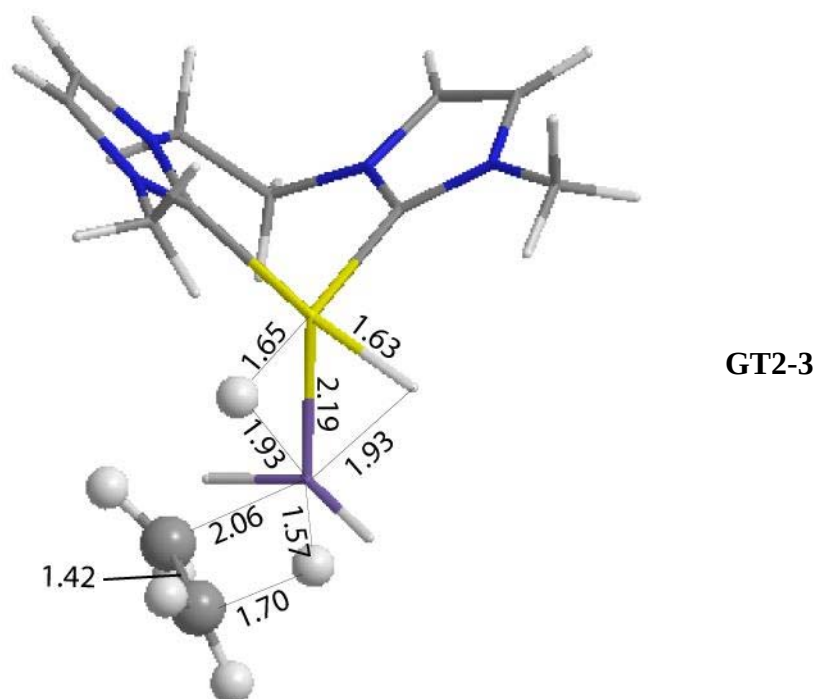
S6. Enthalpy and entropy contributions as well as solvation terms on crucial barriers

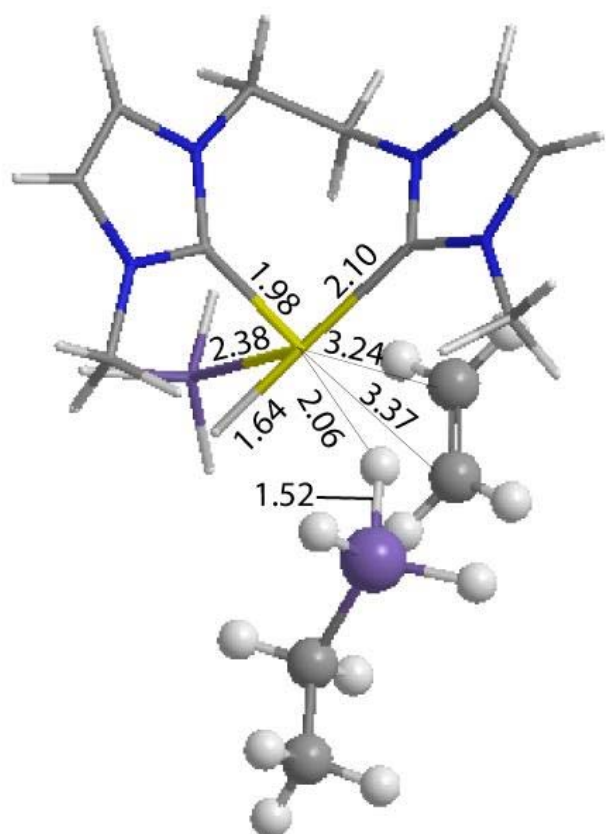
Table S3. Enthalpy ΔH and entropy contributions $-T\Delta S$ as well as solvation effects ΔG_{solv} of crucial activation energies, relative to the preceding intermediates. ΔG_{solv} values determined in single-point fashion at structures optimized in the gas phase, see Computational Details.^[a]

	ΔH	$-T\Delta S$	ΔG_{solv}		ΔH	$-T\Delta S$	ΔG_{solv}
GT2-3	18.5	5.4	-3.2	CH5-6	6.3	0.1	-2.1
GT6-1	37.5	1.8	-1.3	CH2-mCH3	22.3	0.8	-4.1
CH1-2	8.6	0.7	-1.8	SBM5-6S	20.9	-2.2	-0.3
GT4-CH1	9.3	6.8	-0.8	SBM6-CH1	4.0	6.2	-1.5

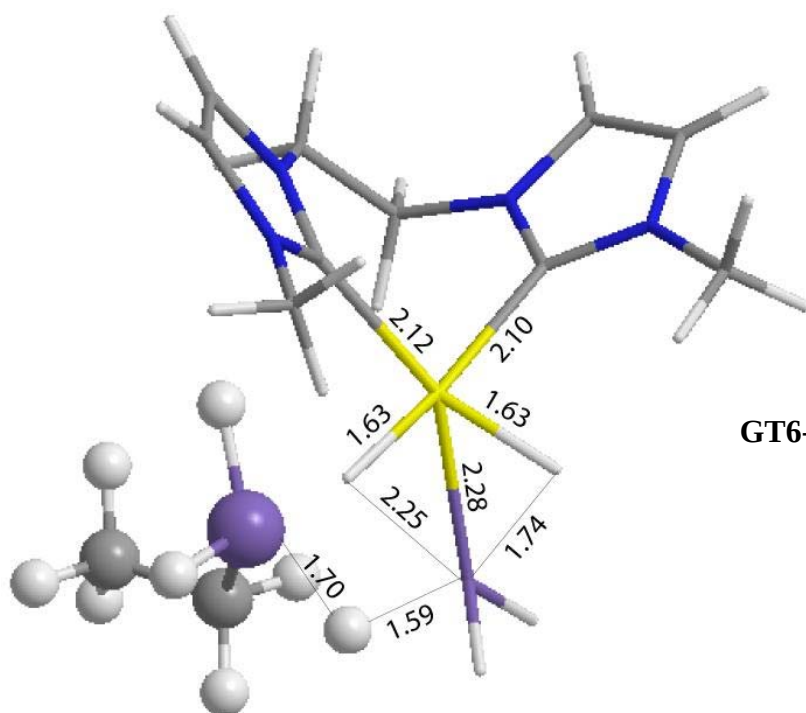
^[a] All values in kcal·mol⁻¹. Temperature $T = 298.15\text{K}$.

S7. Optimized structures for selected intermediates and transition states

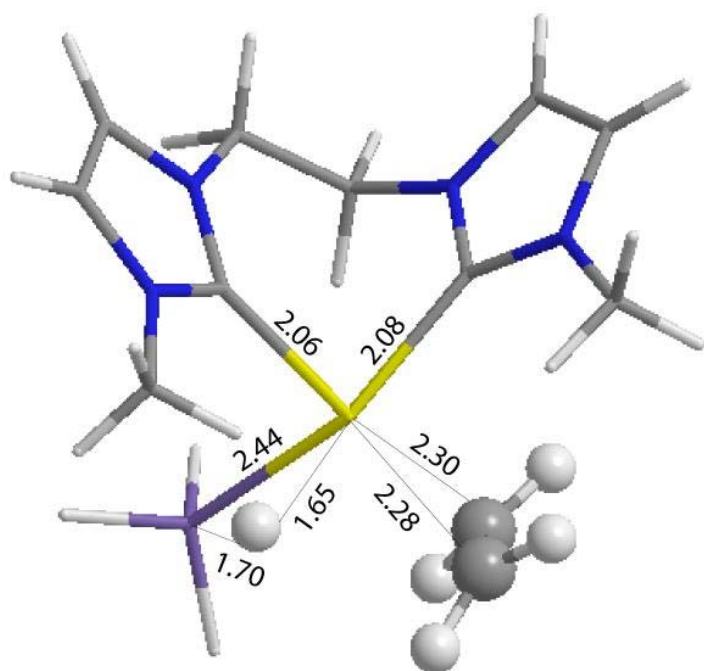




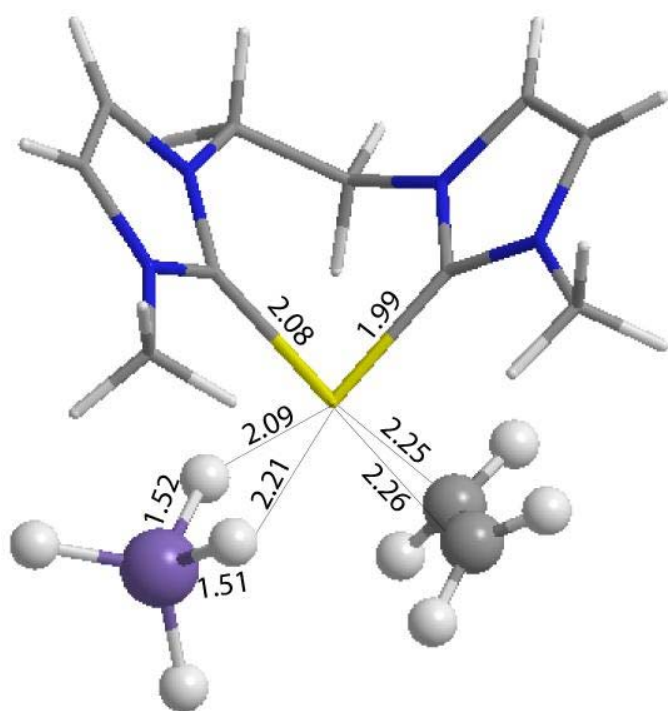
GT4-CH1



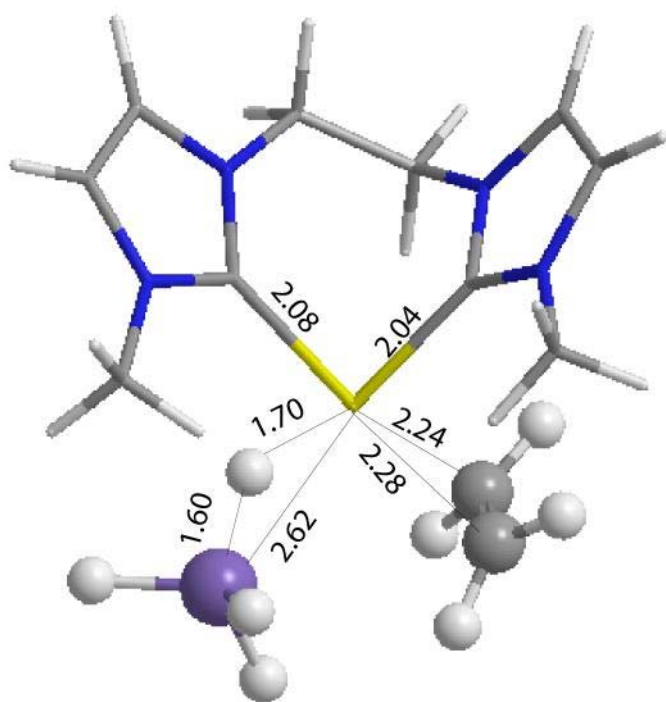
GT6-1



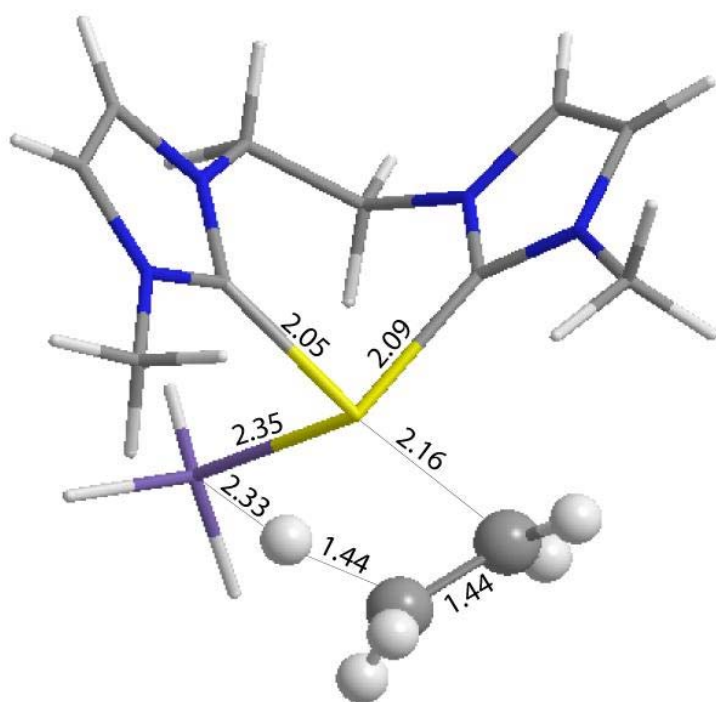
CH1



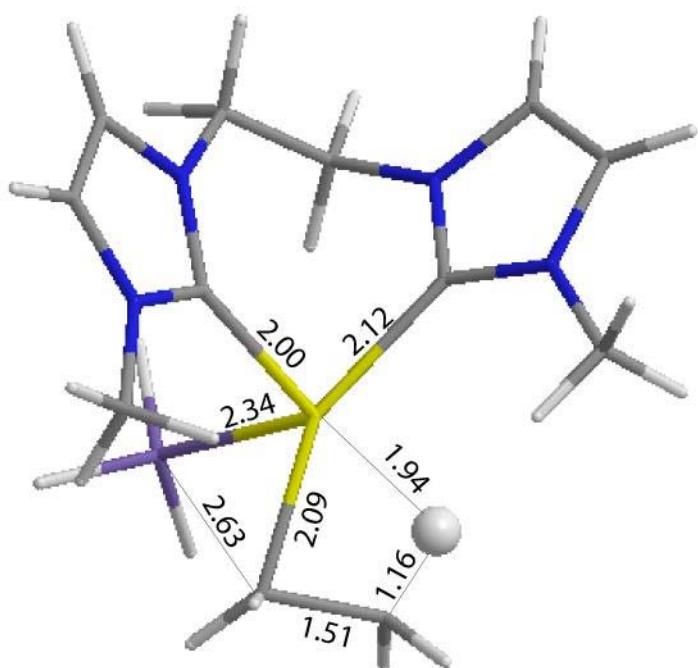
CH1-2



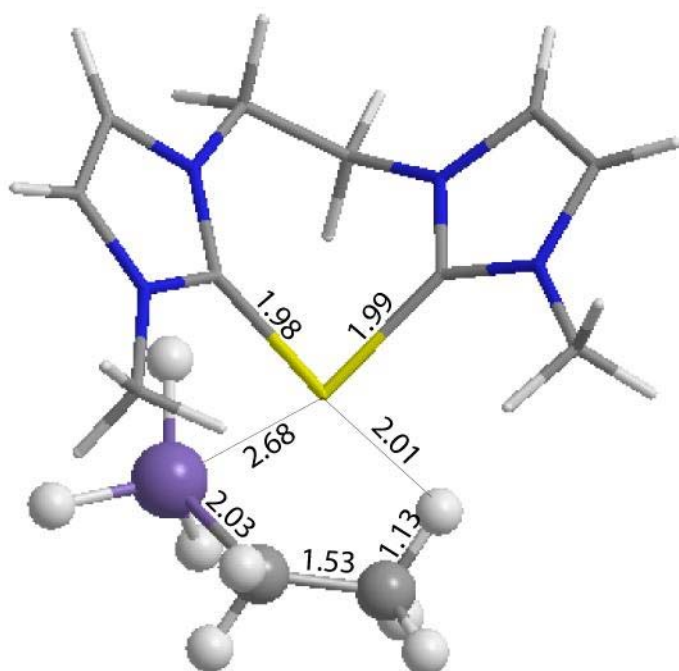
CH2



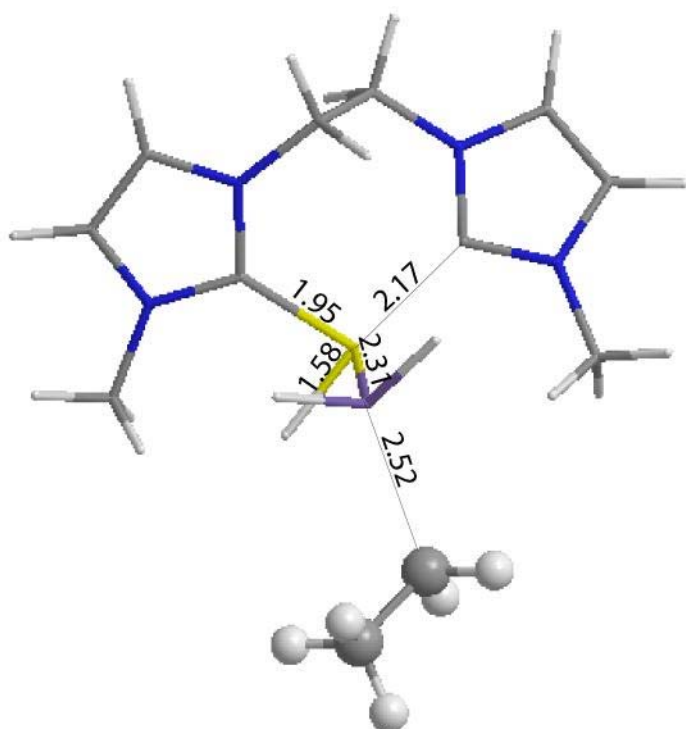
CH1-2b



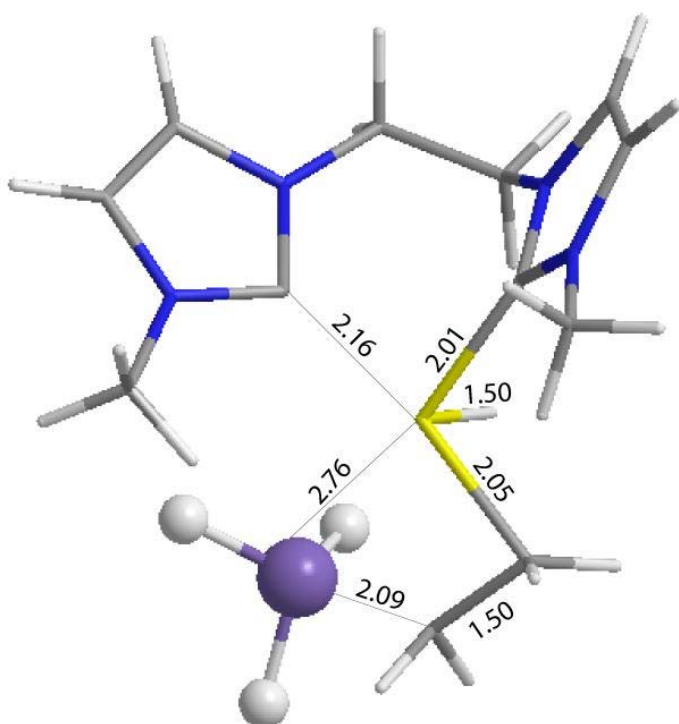
CH5



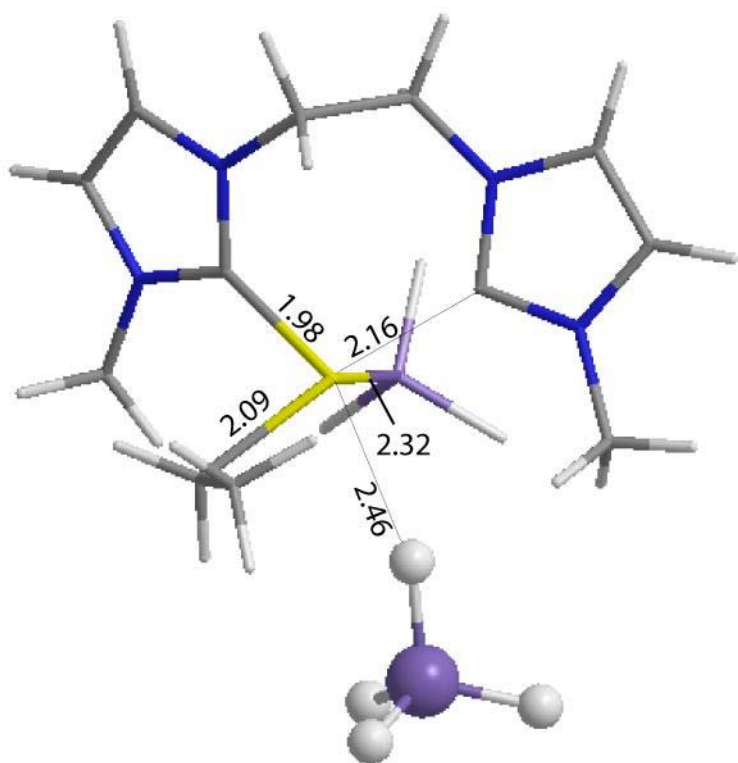
CH5-6



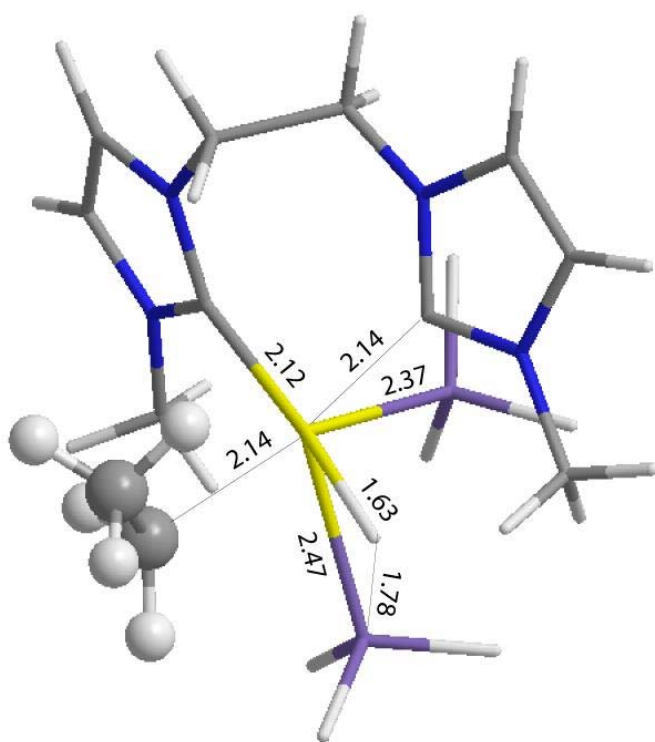
CH4-6*



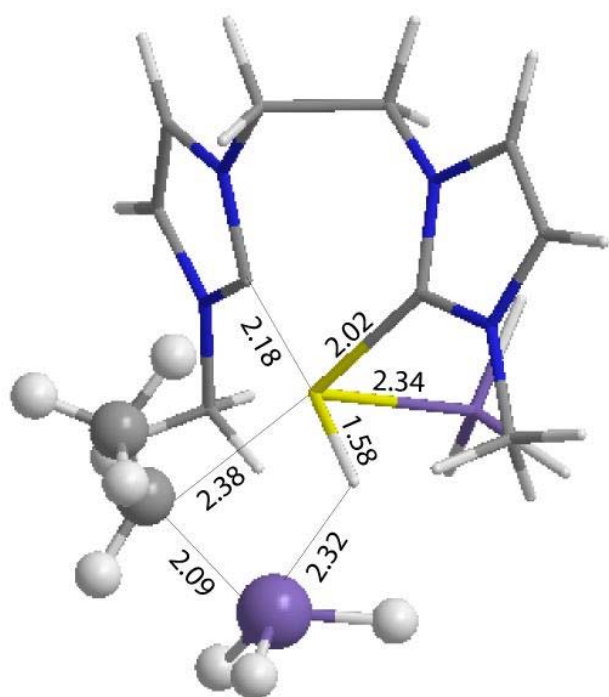
CH2-mCH3



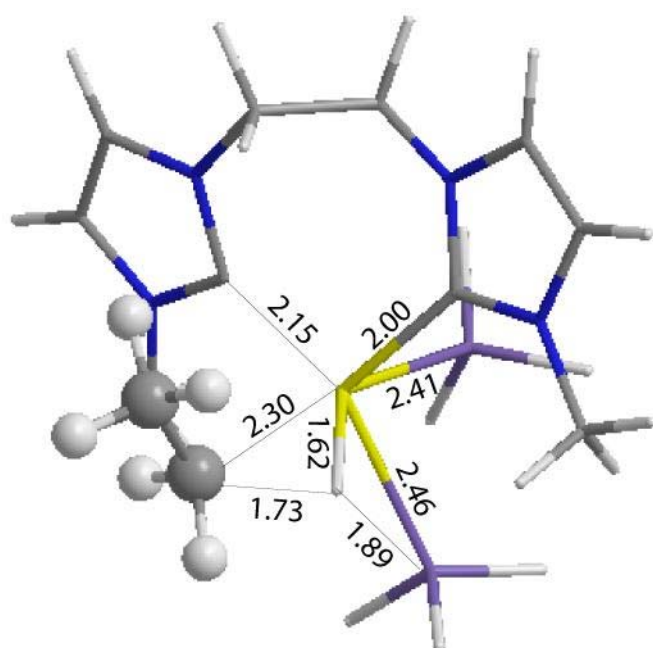
CH4-SBM5



SBM5



SBM5-6



SBM5-6s

S8. Zero-point corrected energies, enthalpies and absolute Gibbs free energies

Table S4. Zero-point corrected energies E_0 , enthalpies H and Gibbs free energies G (in hartree) of all optimized structures.

Code	E_0	H	G
1	-718.641058	-718.625704	-718.683991
2	-291.855029	-291.851020	-291.876592
3	-78.540866	-78.536879	-78.561741
4	-370.437720	-370.431386	-370.465173
GT1	-1010.532874	-1010.514346	-1010.579088
GT2	-1089.078213	-1089.054800	-1089.134342
GT2-3	-1089.046225	-1089.025181	-1089.096040
GT3	-1089.124158	-1089.102369	-1089.175821
GT3-4	-1380.966890	-1380.941124	-1381.024070
GT4	-1380.983857	-1380.958562	-1381.039206
GT4-5	-1380.974860	-1380.949915	-1381.029621
GT5	-1380.987158	-1380.961633	-1381.043242
GT5-6	-1380.975209	-1380.950163	-1381.030336
GT6	-1380.987184	-1380.961767	-1381.043432
GT6-1	-1380.926709	-1380.902333	-1380.981171
CH1	-1089.099465	-1089.077564	-1089.149442
CH1-2	-1089.085465	-1089.063839	-1089.134623
CH2	-1089.093483	-1089.071624	-1089.142910
CH2-3	-1089.085204	-1089.064543	-1089.132530
CH3	-1089.088506	-1089.067330	-1089.136602
CH3-4	-1089.081666	-1089.060919	-1089.128948
CH4	-1089.094999	-1089.073472	-1089.143964
CH4-5	-1089.090049	-1089.069827	-1089.136004
CH5	-1089.091902	-1089.070664	-1089.140346
CH5-6	-1089.081670	-1089.060638	-1089.130114
CH6	-1089.107519	-1089.085931	-1089.157271
CH6-7	-1089.104723	-1089.083583	-1089.154169
CH7	-1089.113472	-1089.091926	-1089.163624
CH7-GT3	-1089.103299	-1089.081904	-1089.154028
GT4-CH1	-1459.510571	-1459.480541	-1459.575195
CH1-2a	-1089.055814	-1089.035041	-1089.103054
CH2a	-1089.059186	-1089.037945	-1089.106886
CH2a-3a	-1089.058182	-1089.037247	-1089.105780
CH3a	-1089.086891	-1089.065507	-1089.135336
CH3a-4	-1089.085420	-1089.064450	-1089.133263
CH1-2b	-1089.078030	-1089.058491	-1089.122826
CH2b	-1089.091440	-1089.070163	-1089.140844
CH2b-6	-1089.081082	-1089.059958	-1089.129972
CH2-mCH3	-1089.057066	-1089.036190	-1089.105748
mCH3	-1089.082404	-1089.061246	-1089.132097
mCH3-CH6	-1089.078878	-1089.057946	-1089.128145
CH3-3a	-1089.084947	-1089.064306	-1089.132398
CH3a-mCH4a	-1089.046399	-1089.025526	-1089.095037

Code	E_0	H	G
mCH4a	-1089.081306	-1089.060455	-1089.130440
mCH4a-CH6	-1089.079283	-1089.058903	-1089.127911
CH3a-mCH4b	-1089.046967	-1089.025968	-1089.096176
mCH4b	-1089.079202	-1089.058519	-1089.127947
mCH4b-5b	-1089.079012	-1089.058890	-1089.126942
mCH5b	-1089.085024	-1089.063816	-1089.134755
mCH5b-CH6	-1089.080196	-1089.059149	-1089.130368
CH4-SBM5	-1380.939689	-1380.914159	-1380.994872
SBM5	-1380.942870	-1380.918753	-1380.993672
SBM5-6	-1380.932187	-1380.908591	-1380.982507
SBM6	-1380.977826	-1380.952816	-1381.032915
SBM6-CH1	-1459.513106	-1459.483261	-1459.578267
SBM5-6S	-1380.910454	-1380.885397	-1380.963795

S9. Complete Reference 47

- [47] Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A., Jr.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. *Gaussian03*, revision B.4; Gaussian, Inc.: Pittsburgh, PA, **2003**.

S10. Geometries

(Cartesian coordinates in Ångstrom)

1

29

Rh	1.1349880	-0.0179300	-0.5647420
C	-0.0345230	1.4136000	0.0094500
N	-0.9700110	1.5888900	0.9905810
C	-1.4322720	2.9036100	0.9910870
C	-0.7735420	3.5613290	0.0083840
N	0.0724470	2.6405420	-0.5877240
C	1.0054250	2.9423430	-1.6707450
H	-0.8287850	4.5890960	-0.3143670
H	-2.1821400	3.2455320	1.6868210
C	0.0207170	-1.4747890	0.0283370
N	-0.2516950	-2.6309000	-0.6433310
C	-1.0263070	-3.4777240	0.1378140
C	-1.2563860	-2.8363800	1.3107950
N	-0.6054330	-1.6115960	1.2307080
C	0.2205280	-2.9512500	-1.9897390
H	-1.3388870	-4.4510770	-0.2061150
H	-1.8093780	-3.1426330	2.1847810
C	-1.5305580	0.5975570	1.9188220
C	-0.6136460	-0.5761330	2.2596580
H	-1.7538920	1.1351760	2.8444980
H	-2.4773300	0.2206720	1.5155600
H	-0.9792130	-1.0367030	3.1801430
H	0.4106200	-0.2369030	2.4298020
H	1.0798480	-3.6263260	-1.9497580
H	-0.5849110	-3.4238510	-2.5552910
H	0.5003830	-2.0199400	-2.4869410
H	0.5376160	3.6297140	-2.3782200
H	1.9262820	3.3896220	-1.2859200
H	1.2315600	2.0129690	-2.2064260

2

5

Si	0.0000030	0.0000470	0.0000200
H	0.3677340	1.0758520	-0.9557870
H	-1.1600230	-0.7597880	-0.5321330
H	-0.3611380	0.6026310	1.3086540
H	1.1533890	-0.9185060	0.1793380

3

6

C	0.0000000	0.0000000	0.6653580
C	0.0000000	0.0000000	-0.6653580
H	0.0000000	0.9235150	1.2382870
H	0.0000000	-0.9235150	1.2382870
H	0.0000000	-0.9235150	-1.2382870
H	0.0000000	0.9235150	-1.2382870

4
11

Si	-1.1566090	-0.1219900	0.0000000
H	-1.3431630	-0.9782920	1.2047770
H	-2.2192490	0.9216990	-0.0000070
H	-1.3431590	-0.9783060	-1.2047670
C	0.5664400	0.6674400	-0.0000010
H	0.6406950	1.3253880	0.8753530
H	0.6406950	1.3253840	-0.8753590
C	1.7235410	-0.3467220	0.0000010
H	2.6967100	0.1566190	0.0000000
H	1.6900520	-0.9944730	-0.8826920
H	1.6900520	-0.9944700	0.8826960

GT1
34

Rh	0.1885500	1.0212200	-0.2697800
C	-3.0141000	-1.6713800	-0.1582400
C	-3.3874700	-0.9212600	0.9091400
H	-3.4884600	-2.5206100	-0.6245700
H	-4.2495100	-0.9929700	1.5534600
C	2.1317800	-2.7587800	0.1080700
C	2.8915300	-1.9882000	0.9208700
H	2.2145800	-3.8012000	-0.1564400
H	3.7658200	-2.2267800	1.5056100
C	1.2411200	-0.6704200	0.0901000
C	-1.4565700	-0.0496000	0.1246200
N	1.1198400	-1.9450500	-0.3923700
N	2.3312000	-0.7213100	0.9077200
N	-1.8269300	-1.1222500	-0.6253900
N	-2.4190600	0.0636000	1.0735100
C	-2.4615000	1.0919100	2.1115500
H	-2.5927700	0.6241400	3.0899100
H	-1.5163800	1.6340100	2.0922200
H	-3.2864700	1.7848900	1.9260500
C	2.8746300	0.4112500	1.6566900
H	3.3618100	0.0383200	2.5590700
H	3.6037400	0.9595000	1.0531800
H	2.0573500	1.0774800	1.9329700
C	0.1238200	-2.5162300	-1.3156300
H	0.6475600	-2.8423800	-2.2209000
H	-0.2885900	-3.4074900	-0.8312700
C	-1.0148200	-1.5956900	-1.7420300
H	-1.6572600	-2.1548000	-2.4272600
H	-0.6323200	-0.7178900	-2.2678100
Si	0.6455800	3.1608100	-1.0077100
H	-0.7656100	2.5475600	-0.5998800
H	0.9477900	4.3199700	-0.1412300
H	0.6567400	3.5570000	-2.4309200
H	1.6931600	2.0004700	-0.7390500

GT2

40

Rh	-0.3825200	-0.5531500	-0.0101300
C	3.7220600	-0.9870100	-0.7231900
C	3.6650200	-1.7559200	0.3933100
H	4.5482000	-0.7475400	-1.3741300
H	4.4336300	-2.3135400	0.9048400
C	1.0416700	3.4776000	0.0011800
C	0.1498500	3.5116400	1.0183800
H	1.6695200	4.2504300	-0.4135700
H	-0.1512900	4.3193900	1.6665100
C	0.1617400	1.3922600	0.2017500
C	1.5751900	-0.9865700	0.0066300
N	1.0463400	2.1752000	-0.4894800
N	-0.3706700	2.2328500	1.1348400
N	2.4316200	-0.5223800	-0.9435700
N	2.3447500	-1.7401400	0.8313600
C	1.8617300	-2.4614500	2.0070300
H	2.4436200	-2.1724900	2.8854800
H	0.8158400	-2.1975700	2.1611600
H	1.9491600	-3.5400400	1.8517800
C	-1.3795300	1.8587700	2.1245400
H	-1.2226500	2.4443600	3.0322300
H	-2.3862300	2.0489600	1.7412700
H	-1.2718400	0.7982800	2.3519600
C	1.9343900	1.8300000	-1.6128300
H	1.6168500	2.4067100	-2.4886400
H	2.9400400	2.1669300	-1.3404700
C	1.9827000	0.3598000	-2.0157100
H	2.6760200	0.2673700	-2.8559100
H	1.0002000	0.0098800	-2.3405400
Si	-2.3401200	-1.7200400	-0.3582600
H	-0.8451800	-2.2878500	-0.1778200
H	-3.1758000	-2.3151700	0.7035000
H	-2.8413300	-2.0708800	-1.7002600
H	-2.1718900	-0.1534700	-0.1508800
C	-5.1951000	0.0560000	-1.2355200
C	-5.6092500	-0.6086700	-0.1537100
H	-5.2489400	-0.3796100	-2.2295200
H	-4.8218200	1.0750900	-1.1735400
H	-5.5912300	-0.1608900	0.8366200
H	-6.0169900	-1.6136600	-0.2216500

GT2-3

40

Rh	0.5854210	-0.4751860	-0.4573230
C	-3.3301740	-1.2279890	1.0517630
C	-3.4916800	-1.8659010	-0.1347140
H	-4.0080850	-1.0973080	1.8806600
H	-4.3417970	-2.3890640	-0.5433410
C	-1.0452870	3.4625700	0.5286030
C	-0.3495710	3.7455320	-0.5970120
H	-1.6490030	4.0928850	1.1626990
H	-0.2405510	4.6669910	-1.1470020
C	-0.0298390	1.5364360	-0.1427170
C	-1.3719200	-1.0649070	-0.0913280

N	-0.8489650	2.1114620	0.7930850
N	0.2605140	2.5663100	-0.9921410
N	-2.0289690	-0.7415080	1.0579080
N	-2.2860610	-1.7568260	-0.8187600
C	-2.0503240	-2.3081930	-2.1511810
H	-2.5692530	-1.7144670	-2.9086430
H	-0.9780910	-2.2885080	-2.3445410
H	-2.4088900	-3.3391750	-2.1913310
C	1.0460290	2.4611570	-2.2207900
H	0.3885200	2.4639650	-3.0945130
H	1.7349110	3.3066270	-2.2854690
H	1.6089220	1.5288140	-2.1956490
C	-1.4751430	1.5192100	1.9866330
H	-1.0111170	1.9639970	2.8745680
H	-2.5267760	1.8241490	1.9783450
C	-1.3864070	0.0037410	2.1336140
H	-1.8710660	-0.2620350	3.0772920
H	-0.3455960	-0.3205150	2.1792000
Si	2.3238930	-1.5403410	0.3530250
H	0.9182240	-2.0128770	-0.8795920
H	3.5803210	-1.8695990	-0.5265410
H	2.3823230	-2.8198270	1.1041530
H	2.1268450	0.0481840	-0.7320290
C	3.6123960	-0.5230220	1.5936200
C	4.4966680	-0.9768890	0.5867020
H	3.6392360	-1.0174050	2.5594470
H	3.3390010	0.5264860	1.5992060
H	4.8127920	-0.3146720	-0.2142470
H	5.1165660	-1.8550450	0.7447300

GT3

40

Rh	-0.5887500	-0.1723700	0.2017300
C	2.9400600	-2.1784500	-0.8320000
C	2.7651400	-2.7609200	0.3808800
H	3.6988600	-2.3277900	-1.5840100
H	3.3445100	-3.5146900	0.8903700
C	2.1721500	3.0180100	-0.4843000
C	1.4952300	3.4801300	0.5924200
H	2.9729800	3.4579100	-1.0575400
H	1.5908600	4.4018600	1.1442500
C	0.6414800	1.4377300	0.0844900
C	1.0601600	-1.3055800	0.0886700
N	1.6464300	1.7649600	-0.7855200
N	0.5734100	2.5035500	0.9332800
N	1.8858400	-1.2881400	-0.9930100
N	1.6135800	-2.2106500	0.9345300
C	1.0722400	-2.5815300	2.2402100
H	1.8440200	-2.4729700	3.0058200
H	0.2412400	-1.9135200	2.4650200
H	0.7184900	-3.6159000	2.2249100
C	-0.3637200	2.6315600	2.0482400
H	0.1056300	3.2146600	2.8425800
H	-1.2816400	3.1318500	1.7261400
H	-0.6046500	1.6358400	2.4201500
C	2.1938400	1.0064400	-1.9232400
H	1.9996200	1.5771100	-2.8381700

H	3.2792300	0.9591500	-1.7858400
C	1.6449700	-0.4016400	-2.1265500
H	2.1301700	-0.8252500	-3.0098900
H	0.5669700	-0.3782100	-2.3021000
Si	-2.8707500	-0.5570200	0.2905000
H	-1.6672500	-1.6189500	0.3258100
H	-5.8338700	0.0488700	-0.2317600
H	-3.5866600	-0.6217000	1.5874600
H	-2.1176700	0.8497400	0.2011600
C	-4.0434400	-0.8401600	-1.1454700
C	-5.2487700	0.1232500	-1.1539200
H	-4.3940100	-1.8790700	-1.0711800
H	-3.4809500	-0.7703700	-2.0831300
H	-4.9341300	1.1656300	-1.2698600
H	-5.9182400	-0.1105500	-1.9865800

GT3-4

45

Rh	-0.4016010	-0.1103920	0.1050960
C	3.5079370	-1.6288620	-0.0722080
C	3.2757600	-1.9313300	1.2303990
H	4.3709310	-1.8048000	-0.6950550
H	3.8988950	-2.4227580	1.9609200
C	1.9673100	3.2323770	-0.9312930
C	1.1412800	3.7960880	-0.0227440
H	2.7664760	3.6567420	-1.5182070
H	1.0804090	4.8083350	0.3441080
C	0.5687800	1.5997220	-0.1801570
C	1.4087720	-0.9309820	0.4363340
N	1.6179100	1.8872400	-1.0200970
N	0.3025000	2.7913660	0.4346410
N	2.3520390	-1.0185310	-0.5416890
N	1.9899470	-1.4917730	1.5277850
C	1.3546170	-1.6357810	2.8358460
H	1.9993520	-1.2122390	3.6095240
H	0.4090560	-1.0941140	2.8150940
H	1.1686290	-2.6903660	3.0555450
C	-0.7201400	3.0138900	1.4526850
H	-0.4353210	3.8810160	2.0506160
H	-1.6941310	3.2012270	0.9929120
H	-0.7848170	2.1357090	2.0933670
C	2.3589710	1.0316120	-1.9628300
H	2.1159590	1.3487320	-2.9834250
H	3.4218870	1.2349460	-1.7976310
C	2.1138440	-0.4713420	-1.8727800
H	2.7872890	-0.9623180	-2.5804790
H	1.0867550	-0.7126160	-2.1512930
Si	-2.7819470	0.0117710	0.7689810
H	-2.0973170	-1.2286350	1.3000330
H	-5.3285030	1.5724150	-0.0104970
H	-3.0513840	0.9745630	1.8650190
H	-1.8879170	0.7125700	-0.3691490
C	-4.3710760	-0.3977100	-0.1564400
C	-5.0702660	0.8293360	-0.7723620
H	-5.0414420	-0.8951060	0.5573560
H	-4.1473710	-1.1407770	-0.9313900
H	-4.4381550	1.3210430	-1.5199210

H	-5.9992390	0.5381350	-1.2714200
Si	-1.2373610	-3.3756590	-1.2799580
H	-2.6943060	-3.5113540	-1.5131200
H	-0.4665980	-3.7735100	-2.4829380
H	-0.8179230	-4.1764170	-0.1048320
H	-0.9303720	-1.9185630	-1.0019560

GT4
45

Rh	-0.4305420	-0.3063930	0.1437330
C	3.5421320	-1.5548490	-0.3794460
C	3.3863910	-2.0245280	0.8833010
H	4.3871430	-1.5955700	-1.0486780
H	4.0722350	-2.5481720	1.5304250
C	1.9588550	3.2478320	-0.7177390
C	1.2302850	3.6940850	0.3304490
H	2.7216820	3.7330910	-1.3060120
H	1.2368630	4.6425730	0.8439150
C	0.5661010	1.5598300	-0.0931970
C	1.4258850	-1.0760470	0.2798190
N	1.5536140	1.9394860	-0.9605900
N	0.3955690	2.6529060	0.7047070
N	2.3306080	-0.9749300	-0.7348760
N	2.0849300	-1.7232220	1.2721820
C	1.5219910	-2.0728130	2.5755700
H	2.0953240	-1.5916030	3.3718400
H	0.4907100	-1.7239550	2.6079980
H	1.5458360	-3.1564210	2.7142790
C	-0.5054810	2.7494460	1.8526020
H	0.0052640	3.2717320	2.6642100
H	-1.4139250	3.2952920	1.5876690
H	-0.7626030	1.7465000	2.1899480
C	2.2134760	1.1724770	-2.0295390
H	1.8644090	1.5421020	-3.0002720
H	3.2816130	1.3980990	-1.9547860
C	2.0059620	-0.3397250	-2.0092210
H	2.6434430	-0.7722540	-2.7850920
H	0.9725270	-0.5885620	-2.2476220
Si	-3.0743440	0.5302570	0.6684740
H	-2.6908800	0.2136910	2.0656280
H	-5.1530800	0.8360710	-1.5874160
H	-3.3550130	1.9855340	0.5670190
H	-1.9207250	0.4389710	-0.3978810
C	-4.5210050	-0.4942060	0.0395580
C	-4.9143330	-0.2198340	-1.4233390
H	-5.3621690	-0.2627840	0.7073940
H	-4.3035750	-1.5576000	0.1884620
H	-4.1102790	-0.4918930	-2.1153150
H	-5.7970600	-0.8025320	-1.7027210
Si	-1.0956780	-2.3456490	-0.9515690
H	-1.1107760	-1.6808900	0.6962670
H	-2.5144200	-2.7774530	-0.8840420
H	-0.2393600	-3.5246780	-0.6654270
H	-0.8430720	-1.9358050	-2.3673210

GT4-5

45

Rh	-0.3769760	-0.3847840	0.2356500
C	3.5956240	-1.2656390	-0.6924980
C	3.6045680	-1.7692340	0.5666340
H	4.3722870	-1.2194230	-1.4396490
H	4.3925450	-2.2432250	1.1303150
C	1.6495050	3.3528670	-0.6948520
C	1.0292600	3.6970960	0.4567420
H	2.3049810	3.9159110	-1.3403220
H	1.0413720	4.6180040	1.0179210
C	0.4501790	1.5477200	-0.0042820
C	1.5198210	-0.9824180	0.1809150
N	1.2968920	2.0340380	-0.9614280
N	0.3119720	2.5856150	0.8708380
N	2.3104140	-0.7878290	-0.9152910
N	2.3281960	-1.5863250	1.0893830
C	1.9302130	-2.0072600	2.4314570
H	2.6100180	-1.5767450	3.1705340
H	0.9181160	-1.6492700	2.6146360
H	1.9526310	-3.0973570	2.5078200
C	-0.4470290	2.5656730	2.1228590
H	0.0453410	3.2243010	2.8401810
H	-1.4716770	2.9093030	1.9631340
H	-0.4603250	1.5519120	2.5199540
C	1.8627610	1.3573610	-2.1393650
H	1.3462270	1.7103250	-3.0390400
H	2.9047400	1.6837000	-2.2071130
C	1.8017650	-0.1701100	-2.1354620
H	2.3931990	-0.5291170	-2.9821350
H	0.7761220	-0.5136600	-2.2692750
Si	-0.9231990	-2.6090210	-0.6297880
H	-0.6790590	-2.3470650	-2.0784990
H	-0.8626970	-1.7910500	0.9032880
H	-0.0238070	-3.7183190	-0.2230690
H	-2.0950000	0.2731300	1.3743520
Si	-2.9715280	0.5283900	0.1619330
H	-3.1826000	1.9914340	0.0476630
H	-2.3298570	-3.0684140	-0.4986370
H	-2.0186300	0.1229750	-0.9562020
C	-4.5565520	-0.4867300	0.1838720
H	-5.1288520	-0.1814920	1.0690480
H	-4.2907130	-1.5387160	0.3399100
C	-5.4133690	-0.3276290	-1.0869660
H	-6.3353070	-0.9109100	-1.0044810
H	-4.8813060	-0.6761700	-1.9780220
H	-5.7004510	0.7153830	-1.2554410

GT5

45

Rh	-0.2804840	-0.4925880	0.4041060
C	3.6649840	-0.7190380	-1.0655990
C	3.9139790	-1.2643670	0.1512520
H	4.3218230	-0.5201710	-1.8979100
H	4.8314400	-1.6278640	0.5865980
C	0.9653940	3.5621810	-0.5360510

C	0.3466150	3.7485200	0.6533520
H	1.4706720	4.2589260	-1.1862440
H	0.2130630	4.6381670	1.2483520
C	0.1645590	1.5452860	0.1357930
C	1.7013360	-0.8092540	0.0663560
N	0.8545270	2.2089160	-0.8391810
N	-0.1293670	2.5101260	1.0523280
N	2.3035410	-0.4455940	-1.1004760
N	2.7018730	-1.3107940	0.8320310
C	2.5497180	-1.8401750	2.1871270
H	3.2236240	-1.3139710	2.8672700
H	1.5200600	-1.6825160	2.5047350
H	2.7786530	-2.9086140	2.2018550
C	-0.8536840	2.2976940	2.3067690
H	-0.4529900	2.9706190	3.0668160
H	-1.9203810	2.4968010	2.1731050
H	-0.7118360	1.2666910	2.6295390
C	1.4405800	1.6896280	-2.0858750
H	0.8356900	2.0372760	-2.9309140
H	2.4310100	2.1459810	-2.1782820
C	1.5631150	0.1711880	-2.1966890
H	2.0781870	-0.0516210	-3.1350370
H	0.5794380	-0.2984120	-2.2342940
Si	-0.5802400	-2.8014610	-0.3861670
H	-0.3407140	-2.5222990	-1.8312680
H	-0.5311990	-1.9472500	1.1043550
H	0.4161180	-3.8202300	0.0323810
H	-1.8734150	-0.2150490	0.9614680
Si	-2.7739420	0.1399820	-0.3155520
H	-3.0203210	1.5909130	-0.1128780
H	-1.9392730	-3.3812650	-0.2481790
H	-2.2928100	-0.0685960	-1.7052000
C	-4.3204680	-0.8790670	0.0445700
H	-4.6182920	-0.6993330	1.0854050
H	-4.0635800	-1.9432640	-0.0191850
C	-5.4856980	-0.5525370	-0.9099000
H	-6.3646020	-1.1581640	-0.6689210
H	-5.2225070	-0.7572230	-1.9528780
H	-5.7841460	0.4987380	-0.8409160

GT5-6

45

Rh	-0.3139460	-0.5044610	0.3332430
C	3.4970510	-0.5382510	-1.5319530
C	3.8884290	-1.1794310	-0.4025820
H	4.0543960	-0.2473100	-2.4085150
H	4.8539590	-1.5561820	-0.1038800
C	0.9223620	3.5386600	-0.0860170
C	0.4198360	3.5602070	1.1697310
H	1.3771990	4.3172830	-0.6777350
H	0.3558830	4.3595880	1.8908320
C	0.1572080	1.4495550	0.3759870
C	1.6684420	-0.7792440	-0.2065690
N	0.7600600	2.2421350	-0.5660360
N	-0.0359200	2.2797670	1.4413120
N	2.1360090	-0.3021810	-1.3928880
N	2.7602380	-1.3123580	0.4003820

C	2.7815430	-1.9478510	1.7173460
H	3.6433860	-1.5843660	2.2807570
H	1.8693790	-1.6825890	2.2491590
H	2.8465320	-3.0347290	1.6197450
C	-0.6630110	1.9033630	2.7078240
H	-0.2379870	2.5127140	3.5072110
H	-1.7435030	2.0658150	2.6640300
H	-0.4640970	0.8505900	2.9035090
C	1.1616840	1.9275950	-1.9480480
H	0.4387620	2.3804410	-2.6361220
H	2.1251280	2.4212700	-2.1082810
C	1.2820910	0.4465720	-2.3079650
H	1.7026100	0.3811360	-3.3151450
H	0.3023920	-0.0315990	-2.3147070
Si	-0.7907400	-3.1371630	0.4187670
H	-0.8758710	-2.2301740	-0.7939730
H	-0.4039870	-2.1515830	1.5191480
H	0.2905930	-4.1255730	0.2309380
H	-1.8115450	-0.2106790	0.9903400
Si	-2.5385880	0.3093010	-0.4564630
H	-2.8647880	1.6866510	0.0034950
H	-2.1039270	-3.7388450	0.7176500
H	-2.0839180	0.4292680	-1.8761730
C	-4.0856250	-0.7784590	-0.4002640
H	-4.4320120	-0.8443470	0.6391570
H	-3.8150380	-1.8001930	-0.6957530
C	-5.2137350	-0.2495170	-1.3063560
H	-6.0927080	-0.8998860	-1.2570240
H	-4.9003190	-0.2013470	-2.3546160
H	-5.5327140	0.7547010	-1.0084300

GT6

45

Rh	-0.3733170	-0.4837740	0.2008300
C	3.4076330	-0.7255280	-1.6933210
C	3.7179670	-1.5775590	-0.6859770
H	3.9926640	-0.3752900	-2.5291590
H	4.6278930	-2.1151800	-0.4710350
C	1.3184020	3.4857280	0.2817620
C	0.7978790	3.4165320	1.5294130
H	1.8635050	4.2738820	-0.2133070
H	0.8064430	4.1295710	2.3386300
C	0.3289740	1.4539440	0.4941880
C	1.5684440	-0.9364030	-0.3752370
N	1.0294150	2.2764590	-0.3430260
N	0.2012510	2.1708540	1.6438750
N	2.0894470	-0.3419240	-1.4848300
N	2.5855820	-1.6898110	0.1148270
C	2.5375780	-2.5324490	1.3095920
H	3.4947040	-2.4672240	1.8302940
H	1.7517170	-2.1714070	1.9706200
H	2.3418230	-3.5733590	1.0408270
C	-0.4923060	1.7204310	2.8514010
H	0.0328760	2.1030240	3.7284130
H	-1.5231410	2.0850920	2.8585280
H	-0.4919370	0.6317110	2.8749090
C	1.4407960	2.0599320	-1.7411690

H	0.8276690	2.6985610	-2.3869850
H	2.4759740	2.4063510	-1.8198030
C	1.3398570	0.6303210	-2.2723700
H	1.7319430	0.6303190	-3.2930590
H	0.3017190	0.2967870	-2.3119290
Si	-1.0942600	-2.6603280	1.1417460
H	-0.8732450	-1.9618940	-0.3694320
H	-0.6757650	-2.2525190	2.5138720
H	-0.3827710	-3.9208000	0.8108020
H	-1.8596290	-0.0745710	0.8381090
Si	-2.5679860	0.4646170	-0.5869800
H	-2.9372380	1.7994800	-0.0426960
H	-2.5528500	-2.9106210	1.1238010
H	-1.9612750	0.7047340	-1.9304190
C	-4.0876940	-0.6428350	-0.7365600
H	-4.5084370	-0.8010740	0.2643810
H	-3.7731510	-1.6307110	-1.0948470
C	-5.1561070	-0.0514360	-1.6769960
H	-6.0238300	-0.7148160	-1.7442620
H	-4.7695110	0.0859410	-2.6923690
H	-5.5138400	0.9206690	-1.3222520

GT6-1

45

Rh	0.0216850	-0.5300520	-0.8280710
C	-2.8727600	-0.9313450	2.3083080
C	-3.5974180	-1.5603590	1.3496100
H	-3.0996530	-0.7234020	3.3422820
H	-4.5810610	-2.0015850	1.3855070
C	-0.9542730	3.4889320	0.5485090
C	-0.8781610	3.6830870	-0.7886570
H	-1.1879750	4.1727400	1.3493880
H	-1.0492560	4.5652540	-1.3851900
C	-0.3653170	1.5046620	-0.3944920
C	-1.6192280	-0.9718890	0.4109870
N	-0.6464990	2.1522580	0.7782340
N	-0.5196660	2.4674730	-1.3477090
N	-1.6683210	-0.5771040	1.7142810
N	-2.8185440	-1.5725030	0.1977890
C	-3.2549580	-2.1697080	-1.0628540
H	-4.1873180	-1.7049540	-1.3927380
H	-2.4840210	-1.9990530	-1.8126200
H	-3.4106950	-3.2443130	-0.9369390
C	-0.4185340	2.2660940	-2.7937040
H	-1.4131220	2.1371140	-3.2292280
H	0.0639470	3.1361890	-3.2434460
H	0.1769950	1.3742610	-2.9825650
C	-0.6118540	1.6504280	2.1617390
H	0.2673140	2.0706460	2.6637900
H	-1.4990230	2.0523900	2.6610700
C	-0.5668180	0.1354440	2.3466960
H	-0.5920130	-0.0640040	3.4217020
H	0.3595490	-0.2771140	1.9469720
Si	1.5427230	-2.1604010	-1.3237800
H	-0.1908620	-2.0652640	-1.3455580
H	1.9330570	-2.4563640	-2.7219060
H	1.7128460	-3.3702420	-0.4786100
H	1.1988280	0.0039860	-1.8134370

Si	2.9115300	-0.0860940	-0.0698470
H	3.5467810	0.6357980	-1.1932530
H	2.9575070	-1.5433430	-0.9337670
H	2.0746170	0.8484740	0.7214380
C	4.1058160	-0.8818750	1.1633610
H	4.8649550	-1.4447540	0.6069750
H	3.5586820	-1.6231940	1.7614340
C	4.7656690	0.1616220	2.0844700
H	5.4391410	-0.3242400	2.7972400
H	4.0235920	0.7204660	2.6651100
H	5.3600460	0.8863540	1.5183190

CH1 40

Rh	0.1178610	1.0034330	0.0379430
C	-2.8404410	-1.9605360	-0.6890820
C	-3.3763680	-1.5143880	0.4739550
H	-3.1618630	-2.7402740	-1.3617530
H	-4.2546530	-1.8318310	1.0137620
C	2.1027200	-2.8102470	0.0754500
C	2.6962030	-2.2146890	1.1357400
H	2.2371510	-3.7928370	-0.3487100
H	3.4434480	-2.5786060	1.8231210
C	1.2239360	-0.7240240	0.2630630
C	-1.5386100	-0.2560190	0.0609360
N	1.1985170	-1.8919920	-0.4502280
N	2.1474280	-0.9462230	1.2394230
N	-1.7166430	-1.1783920	-0.9242140
N	-2.5645450	-0.4758170	0.9216490
C	-2.8033290	0.2545510	2.1658420
H	-3.0375560	-0.4533000	2.9636680
H	-1.8981560	0.7992540	2.4302730
H	-3.6360480	0.9537290	2.0505170
C	2.5506130	0.0194230	2.2630010
H	2.7584520	-0.5127830	3.1930060
H	3.4465520	0.5605880	1.9466960
H	1.7381860	0.7266530	2.4239630
C	0.4246790	-2.2448750	-1.6536590
H	1.1037270	-2.2572360	-2.5137040
H	0.0647140	-3.2671540	-1.5021110
C	-0.7530960	-1.3367110	-2.0080490
H	-1.2611620	-1.7762460	-2.8707260
H	-0.4068350	-0.3409550	-2.2890720
Si	1.9501070	1.8696060	-1.3274980
H	1.9441570	3.3304620	-1.5968200
H	1.5255800	1.1724210	-2.5785150
H	3.3386960	1.4340900	-1.0313480
C	-1.2150210	2.6467490	-0.8501670
C	-0.9392600	2.9742810	0.4581210
H	-0.6721530	3.1113900	-1.6682110
H	-2.1448400	2.1593530	-1.1240600
H	-1.6485720	2.7605380	1.2513570
H	-0.1753990	3.7056650	0.7002320
H	1.4458720	1.9539790	0.2886360

CH1-2

40

Rh	-0.4598110	-0.8433050	-0.1241370
C	3.4210430	0.6263100	-0.4427610
C	3.5846270	0.0429880	0.7701310
H	4.1127500	1.1790370	-1.0589750
H	4.4467470	-0.0099100	1.4161940
C	-0.6111480	3.4574280	-0.1462980
C	-1.3884260	3.2169460	0.9341910
H	-0.3042880	4.3853760	-0.6024920
H	-1.8870050	3.8932400	1.6104460
C	-0.7450310	1.2000430	0.1053190
C	1.4535110	-0.3658220	0.1187250
N	-0.2146300	2.2184150	-0.6413890
N	-1.4532330	1.8390940	1.0803740
N	2.1122540	0.3651210	-0.8285110
N	2.3714960	-0.5544640	1.1040320
C	2.1333160	-1.2449140	2.3697800
H	2.4732580	-0.6178980	3.1972790
H	1.0630880	-1.4221660	2.4672460
H	2.6705380	-2.1968670	2.3971450
C	-2.1752570	1.1930260	2.1764690
H	-2.0612740	1.7945600	3.0803240
H	-3.2383610	1.0982680	1.9399670
H	-1.7507540	0.2046940	2.3456970
C	0.6637660	2.1509880	-1.8217190
H	0.0695740	2.3364630	-2.7237360
H	1.3734500	2.9770740	-1.7188990
C	1.4313060	0.8409390	-2.0267100
H	2.1714090	1.0059520	-2.8147200
H	0.7551550	0.0462110	-2.3472280
Si	-3.1132700	-1.2946540	-0.6487380
H	-3.6333170	-2.6266070	-1.0212130
H	-1.9679090	-0.8999870	-1.5621630
H	-4.1393080	-0.2317210	-0.6463750
C	0.1358810	-2.7797020	-1.1096640
C	-0.1230180	-3.0486350	0.2210830
H	-0.6020980	-2.9920640	-1.8777500
H	1.1541970	-2.6627910	-1.4678890
H	0.6858870	-3.1592240	0.9348620
H	-1.0703680	-3.4815530	0.5286980
H	-2.4387340	-1.3609110	0.6992560

CH1-2a

40

Rh	-0.0526700	-0.8970800	-0.1497300
C	-2.4168200	2.6025600	0.1421700
C	-3.2734500	1.7543500	-0.4632500
H	-2.5223000	3.6396100	0.4175100
H	-4.2785900	1.9022300	-0.8242500
C	3.2960000	1.7948800	-0.4510600
C	3.8751000	0.5727300	-0.4252100
H	3.7265900	2.7819100	-0.5040900
H	4.9131500	0.2816000	-0.4433400
C	1.6261400	0.2584300	-0.3375800
C	-1.3691100	0.5876700	-0.0307700

N	1.9216600	1.5874900	-0.3922900
N	2.8483100	-0.3554200	-0.3584800
N	-1.2558700	1.8832400	0.4060500
N	-2.6286000	0.5289500	-0.5754300
C	-3.2117500	-0.5534900	-1.3704300
H	-4.0344800	-0.1362400	-1.9510600
H	-2.4630900	-0.9419800	-2.0596400
H	-3.6030700	-1.3545700	-0.7436800
C	3.0718600	-1.7991200	-0.3090900
H	4.1268800	-1.9955000	-0.5022300
H	2.8129200	-2.1994200	0.6744700
H	2.4704100	-2.2876200	-1.0793800
C	0.9692100	2.6938900	-0.3431000
H	1.5582400	3.6033700	-0.2090600
H	0.4387600	2.7788600	-1.2967500
C	-0.0282500	2.5620200	0.8144400
H	-0.3243800	3.5561100	1.1541100
H	0.4285900	2.0452200	1.6577300
Si	-0.2336200	-0.7477500	2.2702100
H	0.6633800	-1.8757900	2.6729200
H	-1.5632500	-0.9618400	2.9029200
H	0.3305200	0.4794800	2.9026100
C	-1.4212300	-2.6723800	0.4386700
C	-0.9151900	-2.9363700	-0.8229100
H	-0.9743200	-3.1559400	1.3022300
H	-2.4325100	-2.3181100	0.5914400
H	-1.4911800	-2.7888500	-1.7278800
H	-0.0548300	-3.5887500	-0.9383600
H	0.4999000	-1.3274000	-1.6513600

CH1-2b

40

Rh	-0.1849680	-1.0402710	-0.1148850
C	3.0506580	1.7802350	-0.4595260
C	3.5279730	1.0826990	0.6141580
H	3.4558420	2.6354990	-0.9944170
H	4.4338070	1.2102200	1.2013550
C	-1.7203990	2.9063200	0.6427410
C	-2.4203070	2.1646650	1.5499910
H	-1.7093430	3.9774030	0.4573020
H	-3.1202160	2.4640870	2.3258000
C	-1.1523690	0.7122970	0.3162070
C	1.5645700	0.0949030	-0.0124780
N	-0.9545930	2.0150550	-0.1104230
N	-2.0747640	0.8359880	1.3329460
N	1.8550920	1.1622510	-0.8222220
N	2.6087400	0.0652600	0.8784420
C	2.7699660	-0.8810390	1.9868110
H	3.1389130	-0.3419070	2.8724780
H	1.7938670	-1.3247660	2.2229390
H	3.4855130	-1.6764670	1.7225760
C	-2.6007940	-0.2802230	2.1237850
H	-1.8417220	-0.6509510	2.8305340
H	-3.4802550	0.0702310	2.6826480
H	-2.8992840	-1.0965060	1.4498690
C	-0.1894220	2.5271870	-1.2700940
H	-0.8991840	2.7427520	-2.0897650

H	0.2503460	3.4855670	-0.9457690
C	0.9129930	1.6223880	-1.8358330
H	1.4596880	2.1977070	-2.6010640
H	0.4872810	0.7323990	-2.3195540
Si	-1.8129230	-0.8163250	-1.7914660
H	-1.6671860	-2.0243460	-2.6758080
H	-1.6124520	0.3969540	-2.6584980
H	-3.2424100	-0.7569190	-1.3333230
C	0.9468960	-2.8746090	-0.2307080
C	-0.4245760	-3.2995440	-0.1128100
H	1.4460240	-2.9315400	-1.2041910
H	1.6030350	-3.0262050	0.6321080
H	-0.7299820	-3.7675700	0.8337940
H	-0.9105300	-3.7361530	-0.9949900
H	-1.3697550	-2.2203050	0.0116660

CH2

40

Rh	-0.6589940	-0.6513850	-0.2759810
C	3.5181640	-0.2585720	-0.0745590
C	3.3846150	-0.8615380	1.1330400
H	4.3950080	0.0963080	-0.5931720
H	4.1228020	-1.1310070	1.8719730
C	0.3405240	3.5367570	-0.1828960
C	-0.6122350	3.5281410	0.7764650
H	0.9426670	4.3423130	-0.5725600
H	-0.9998300	4.3220040	1.3951250
C	-0.4263810	1.4010680	-0.0057920
C	1.3150170	-0.7163560	0.2300380
N	0.4556300	2.2301740	-0.6484410
N	-1.0624810	2.2202210	0.8785470
N	2.2400160	-0.1802570	-0.6144400
N	2.0289110	-1.1308410	1.3058880
C	1.4671040	-1.7447940	2.5077890
H	1.7577860	-1.1674230	3.3887850
H	0.3814450	-1.7429960	2.4186720
H	1.8266310	-2.7714210	2.6160720
C	-2.0794560	1.8121640	1.8469830
H	-1.9487060	2.3895440	2.7641670
H	-3.0837540	1.9886950	1.4531160
H	-1.9537200	0.7546000	2.0726890
C	1.4327660	1.9258730	-1.7078360
H	1.0340660	2.2647420	-2.6707620
H	2.3179280	2.5292430	-1.4864940
C	1.8409350	0.4590770	-1.8645180
H	2.6760820	0.4170230	-2.5692360
H	1.0134450	-0.1237570	-2.2734280
Si	-3.2758070	-0.8352630	-0.2462020
H	-4.1827840	0.3250790	-0.4224220
H	-3.1934170	-1.1635820	1.1982320
H	-3.7856370	-2.0008590	-1.0056690
C	-0.5049400	-2.5577440	-1.4490810
C	-0.8054160	-2.9182260	-0.1487420
H	-1.2743940	-2.5356580	-2.2150890
H	0.5157450	-2.6068430	-1.8172110
H	-0.0250180	-3.2523320	0.5266690
H	-1.8125220	-3.2110250	0.1323610

H	-2.0665270	-0.3268360	-1.1620650
---	------------	------------	------------

CH2-3
40

Rh	-0.9084740	-0.1989080	-0.5165000
C	2.9336730	-1.8705750	0.3229560
C	2.4153740	-2.2429620	1.5201570
H	3.9223260	-1.9968920	-0.0900110
H	2.8676490	-2.7576640	2.3534100
C	2.0407800	2.8776790	-0.2333290
C	1.1496990	3.4464000	0.6068010
H	3.0089710	3.2134530	-0.5688580
H	1.1905450	4.3712050	1.1594560
C	0.2376410	1.4863550	-0.1007190
C	0.7467650	-1.2450820	0.3633540
N	1.4836800	1.6764930	-0.6563760
N	0.0632570	2.5886860	0.6823060
N	1.8918780	-1.2655770	-0.3720290
N	1.0780150	-1.8493380	1.5267670
C	0.1613610	-2.0865190	2.6411130
H	0.5778380	-1.6682860	3.5605250
H	-0.7853990	-1.5969190	2.4189080
H	-0.0025870	-3.1588900	2.7748590
C	-1.0930700	2.9004720	1.5233000
H	-0.8374940	3.7559510	2.1488220
H	-1.9569940	3.1549920	0.9092590
H	-1.3320990	2.0569660	2.1699890
C	2.2240100	0.8722750	-1.6428640
H	2.0428120	1.2754530	-2.6456770
H	3.2826450	1.0212040	-1.4147540
C	1.9256790	-0.6287830	-1.6808980
H	2.6866900	-1.1084120	-2.3027790
H	0.9585140	-0.8145000	-2.1600670
Si	-2.9031620	0.2723860	0.5809860
H	-3.5459610	1.6037950	0.4560960
H	-2.6068970	0.0745510	2.0351740
H	-3.9226560	-0.7365150	0.1864220
C	-2.0974890	-1.5260680	-1.9147180
C	-1.6423400	-2.3446020	-0.9010580
H	-3.1276040	-1.1931340	-1.9464170
H	-1.5586570	-1.4465250	-2.8562480
H	-0.7555490	-2.9537030	-1.0345160
H	-2.2978410	-2.6407450	-0.0876370
H	-1.9129450	0.7986980	-1.2465170

CH2a
40

Rh	0.0613130	-0.7963150	-0.4392320
C	2.4161100	2.6390870	-0.1034520
C	3.2998370	1.7291760	0.3591860
H	2.5046680	3.7038480	-0.2474000
H	4.3172330	1.8394970	0.6982480
C	-3.3253850	1.7366980	0.3488470
C	-3.8666350	0.5090710	0.1744140
H	-3.7846050	2.6910080	0.5515660

H	-4.8931390	0.1785000	0.1860830
C	-1.6147930	0.2931860	-0.0055880
C	1.3897710	0.6173040	-0.1325630
N	-1.9451430	1.5887570	0.2291410
N	-2.8105710	-0.3642890	-0.0404890
N	1.2495850	1.9472730	-0.4046410
N	2.6642290	0.4937490	0.3468780
C	3.3439250	-0.7072520	0.8362280
H	3.6912220	-1.3269270	0.0072740
H	4.2068760	-0.3885640	1.4205850
H	2.6762240	-1.2758730	1.4804040
C	-2.9652940	-1.7697620	-0.4043560
H	-3.9024600	-2.1490400	0.0055500
H	-2.9721590	-1.8897010	-1.4917920
H	-2.1520800	-2.3520750	0.0398030
C	-1.0223550	2.7226260	0.2459070
H	-1.6263780	3.6179550	0.0836570
H	-0.5469940	2.8123470	1.2280120
C	0.0398630	2.6254630	-0.8557380
H	0.3406900	3.6308920	-1.1551130
H	-0.3559490	2.1101760	-1.7339490
Si	-0.0879960	-1.4044390	1.9901490
H	0.9592110	-2.3144890	2.5496560
H	-1.3930490	-2.0596110	2.3174530
H	-0.0313790	-0.1757860	2.8412290
C	1.2155220	-2.7453110	-0.5479190
C	1.3940560	-2.0651800	-1.7485030
H	1.9950650	-2.8315450	0.1943950
H	0.4428400	-3.5092830	-0.4725420
H	0.7992450	-2.3118480	-2.6215190
H	2.3113860	-1.5267580	-1.9653390
H	-0.0480480	-0.1454950	-1.9279350

CH2a - 3a

40

Rh	0.0282230	-0.8284830	-0.4475220
C	2.4062940	2.5700230	-0.2051520
C	3.2829750	1.7290210	0.3828900
H	2.4939450	3.6106200	-0.4737460
H	4.2902050	1.8884020	0.7334450
C	-3.3154220	1.7667390	0.4179980
C	-3.8762180	0.5353610	0.4047110
H	-3.7487390	2.7407350	0.5806510
H	-4.8968420	0.2205760	0.5543600
C	-1.6602280	0.2770590	-0.0049270
C	1.3923010	0.5414690	-0.0289420
N	-1.9575740	1.5914870	0.1586640
N	-2.8540720	-0.3635870	0.1358970
N	1.2530610	1.8375170	-0.4524640
N	2.6567300	0.4943520	0.4987950
C	3.3595780	-0.6072660	1.1609950
H	4.1472970	-0.9969920	0.5105250
H	3.8089760	-0.2297510	2.0813610
H	2.6665240	-1.4033530	1.4096780
C	-3.0440290	-1.8020430	-0.0280160
H	-4.0352720	-1.9881530	-0.4450920
H	-2.3041130	-2.1821060	-0.7410850

H	-2.9383630	-2.3265730	0.9237120
C	-1.0371770	2.7177490	-0.0070110
H	-1.6388040	3.5647730	-0.3463870
H	-0.5934020	2.9879460	0.9572150
C	0.0621250	2.4484110	-1.0380770
H	0.3828390	3.4009550	-1.4638110
H	-0.3073820	1.8196890	-1.8507200
Si	0.1356180	-1.3050730	1.9622090
H	0.9908080	-2.4643780	2.3577520
H	-1.2594890	-1.6804450	2.3451250
H	0.5301220	-0.1760510	2.8543700
C	1.5220620	-2.4604050	-0.8641240
C	1.0102770	-2.0618230	-2.0955830
H	2.5285630	-2.1776930	-0.5908500
H	1.1444590	-3.3543610	-0.3744010
H	0.2231040	-2.6263380	-2.5852830
H	1.5718650	-1.4045820	-2.7509960
H	-0.5272250	-0.5143280	-1.9730480

CH2b

40

Rh	-0.1025390	-0.8978330	-0.0329130
C	-2.3877120	2.6442720	-0.0573130
C	-3.1518960	1.8849820	-0.8767630
H	-2.5111170	3.6590360	0.2860280
H	-4.0720910	2.1093480	-1.3921260
C	3.2786120	1.9906390	-0.2192270
C	3.8834740	0.8352710	-0.5784610
H	3.6708780	2.9898150	-0.1136320
H	4.9087130	0.6276430	-0.8406600
C	1.6846110	0.3530370	-0.1783570
C	-1.3893080	0.6086250	-0.2317720
N	1.9459630	1.6837660	0.0188930
N	2.9077280	-0.1460250	-0.5523980
N	-1.3139620	1.8533020	0.3284620
N	-2.5358980	0.6457360	-0.9740680
C	-3.1020480	-0.4492410	-1.7628980
H	-3.9207810	-0.0490250	-2.3612700
H	-2.3483520	-0.8636290	-2.4322930
H	-3.4845420	-1.2331320	-1.1085860
C	3.2116920	-1.5404800	-0.8735870
H	2.4980200	-1.9294130	-1.6006940
H	4.2076630	-1.5840360	-1.3152910
H	3.2018520	-2.1589650	0.0270720
C	1.0077550	2.7659060	0.3425810
H	1.5724510	3.4956670	0.9292010
H	0.6936640	3.2594190	-0.5841060
C	-0.2163240	2.3559960	1.1523270
H	-0.5942680	3.2397460	1.6711330
H	0.0472410	1.6177130	1.9083680
Si	-0.8191620	-1.0558680	2.1700600
H	-2.2611660	-0.7570100	2.3776100
H	-0.0424820	-0.1085580	3.0233760
H	-0.5422450	-2.4289440	2.6736400
C	-1.2402350	-2.6352530	-0.1917920
C	0.1029560	-3.3098260	-0.0510850
H	-1.9837200	-2.9456760	0.5440610

H	-1.6628460	-2.7110270	-1.1953950
H	0.4388940	-3.8563170	-0.9358010
H	0.2006700	-3.9300560	0.8424840
H	0.9498030	-2.5389790	0.1089990

CH2b - 6

40

Rh	0.4287400	-0.7308330	-0.0218090
C	0.4463380	3.4320810	0.0198840
C	1.0518790	3.2329630	1.2160340
H	0.1968420	4.3420730	-0.5027180
H	1.4344620	3.9363050	1.9386540
C	-3.7001650	0.2390870	-0.4091460
C	-3.7470840	-0.8226980	0.4267500
H	-4.4897930	0.8405150	-0.8313440
H	-4.5850150	-1.3295590	0.8786630
C	-1.5537810	-0.4170420	-0.0318410
C	0.6063350	1.1908290	0.3446140
N	-2.3572680	0.4842130	-0.6809880
N	-2.4356010	-1.2062260	0.6577020
N	0.1785830	2.1712180	-0.5002770
N	1.1369560	1.8568360	1.4064480
C	1.7430540	1.2346060	2.5808720
H	1.3766910	1.7258810	3.4848650
H	1.4530730	0.1843670	2.6008580
H	2.8329530	1.3156430	2.5416420
C	-2.0706610	-2.3216020	1.5284710
H	-1.0730640	-2.1408990	1.9301590
H	-2.7841550	-2.3797440	2.3526060
H	-2.0820510	-3.2678480	0.9792490
C	-2.0019690	1.6082320	-1.5634030
H	-2.4352410	1.4159430	-2.5512840
H	-2.4872490	2.5020350	-1.1569360
C	-0.5137090	1.8760900	-1.7495180
H	-0.4099150	2.7376930	-2.4143810
H	-0.0192330	1.0234300	-2.2149950
Si	2.7574480	-0.6985130	-1.3730650
H	4.0137050	-0.1828940	-0.7700790
H	2.1086780	0.4613840	-2.0388330
H	3.0574010	-1.6679240	-2.4569430
C	2.2556340	-2.0736520	0.0512490
C	1.1873950	-3.1062930	-0.3238580
H	3.2606020	-2.4872570	-0.0939380
H	2.2327940	-1.8084630	1.1175540
H	1.0709380	-3.8810710	0.4381160
H	1.4010440	-3.5725550	-1.2884520
H	0.1506920	-2.6782700	-0.4590050

CH3

40

Rh	-0.0047450	-0.8465390	-0.6167450
C	2.4027750	2.6013390	0.2449220
C	2.9509590	1.8711400	1.2462600
H	2.6010630	3.6074850	-0.0897950
H	3.7183300	2.1212700	1.9617150

C	-2.8057140	2.2822480	0.2899990
C	-3.4991300	1.2475360	0.8116100
H	-3.0507340	3.3295980	0.2109200
H	-4.4627500	1.2153780	1.2943760
C	-1.5470670	0.4016200	0.0047380
C	1.4247180	0.5404720	0.2218980
N	-1.6160150	1.7604700	-0.2052980
N	-2.7299200	0.1112170	0.6234110
N	1.4771340	1.7659160	-0.3690920
N	2.3473500	0.6168560	1.2153280
C	2.6731710	-0.4445330	2.1679990
H	1.9653290	-0.4483100	3.0002900
H	2.6452690	-1.4097850	1.6659580
H	3.6797820	-0.2757260	2.5525370
C	-3.2162840	-1.2105230	1.0198640
H	-4.3028930	-1.1638820	1.0999910
H	-2.9483850	-1.9406200	0.2583740
H	-2.8010330	-1.5084470	1.9845150
C	-0.7573190	2.6611610	-0.9947680
H	-1.3220090	2.9670180	-1.8827000
H	-0.5858760	3.5558480	-0.3877710
C	0.5847100	2.1163370	-1.4623890
H	1.0602530	2.8856770	-2.0772760
H	0.4568920	1.2358800	-2.1026900
Si	-0.1424080	-2.4243220	1.0690050
H	-1.1834970	-3.4650540	0.8756360
H	-0.3845880	-1.7638510	2.3833440
H	1.1662960	-3.1352610	1.1468350
C	0.7761250	-2.4649680	-1.9773850
C	1.8681310	-1.7711690	-1.4809110
H	0.5079500	-3.4421840	-1.5888320
H	0.3697010	-2.2384210	-2.9588050
H	2.3457790	-0.9966030	-2.0744430
H	2.4741460	-2.1855520	-0.6828880
H	-1.2221000	-1.6748350	-1.2032950

CH3-4

40

Rh	0.0292300	-0.8181720	-0.5788890
C	2.4612140	2.5728510	0.1063050
C	3.0808530	1.8348790	1.0747070
H	2.6451400	3.5722340	-0.2548500
H	3.9063400	2.0724760	1.7261440
C	-2.8383700	2.3024300	0.3551430
C	-3.5148640	1.2464430	0.8876720
H	-3.0982080	3.3461630	0.2778660
H	-4.4713350	1.1936840	1.3820290
C	-1.5402190	0.4263030	0.0500880
C	1.4456410	0.5123910	0.1797890
N	-1.6431260	1.7913010	-0.1546860
N	-2.7194630	0.1264000	0.6834520
N	1.4716340	1.7434010	-0.4236060
N	2.4550120	0.5886390	1.0937670
C	2.8795590	-0.4716290	2.0075840
H	2.3359930	-0.4109570	2.9536200
H	2.7030700	-1.4398290	1.5466120
H	3.9482070	-0.3641020	2.1987080

C	-3.1655710	-1.2045550	1.0927920
H	-4.2510190	-1.1868700	1.1971440
H	-2.8953140	-1.9322420	0.3295760
H	-2.7224960	-1.4920090	2.0483960
C	-0.7794490	2.6972130	-0.9419570
H	-1.3630770	3.0537490	-1.7976200
H	-0.5458480	3.5623680	-0.3134780
C	0.5213360	2.1027920	-1.4762990
H	0.9883790	2.8480220	-2.1258600
H	0.3346850	1.2194370	-2.0968410
Si	0.0167250	-2.2854120	1.2110690
H	-1.0608720	-3.3007700	1.0740210
H	-0.1688960	-1.5620650	2.4990420
H	1.2926310	-3.0508670	1.2838850
C	0.1868050	-2.5483500	-2.0120880
C	1.4645150	-2.0340920	-1.6435270
H	-0.1236540	-3.5190740	-1.6332630
H	-0.2089030	-2.3287740	-3.0014690
H	1.9988560	-1.4100290	-2.3567050
H	2.1062750	-2.6264240	-0.9987830
H	-1.0565630	-1.7988260	-1.3168990

CH3a

40

Rh	-0.0855500	-0.8448400	-0.4355800
C	2.8677600	2.3668800	-0.2272400
C	3.5998500	1.4526100	0.4507900
H	3.0984400	3.3752500	-0.5329200
H	4.6001100	1.5042800	0.8511700
C	-2.9483200	2.2888000	0.3246100
C	-3.7696200	1.2150100	0.3305900
H	-3.1599000	3.3408000	0.4299200
H	-4.8407900	1.1497100	0.4331700
C	-1.6479700	0.4348800	0.0426500
C	1.5920000	0.4830200	-0.0180600
N	-1.6611500	1.8047500	0.1472600
N	-2.9757400	0.0964700	0.1555700
N	1.6523700	1.7555500	-0.5075400
N	2.8113900	0.3149000	0.5738400
C	3.3078400	-0.8696700	1.2735400
H	4.0829000	-1.3647700	0.6821600
H	3.7300800	-0.5681000	2.2345500
H	2.4912200	-1.5614700	1.4562900
C	-3.5888400	-1.2291700	0.0089300
H	-4.6298400	-1.1501500	0.3241000
H	-3.5528700	-1.5525700	-1.0329300
H	-3.0856300	-1.9592700	0.6375700
C	-0.5295600	2.7363000	0.1088500
H	-0.9674100	3.7270700	-0.0271500
H	-0.0157100	2.7334500	1.0750200
C	0.4883100	2.4729000	-1.0122500
H	0.8431800	3.4239900	-1.4146300
H	0.0295300	1.9187100	-1.8347300
Si	-0.2556300	-1.6956200	1.7009700
H	0.5141400	-2.9749300	1.7483100
H	-1.6388100	-1.9896100	2.1594900
H	0.3451600	-0.7603400	2.6922700

C	0.3768700	-2.7825700	-1.5526700
C	1.5706900	-2.1155800	-1.3582700
H	0.0995500	-3.6248100	-0.9282900
H	-0.1561100	-2.7088100	-2.4962400
H	2.0010900	-1.5084000	-2.1499400
H	2.2551400	-2.4420400	-0.5860200
H	-1.3169400	-1.7735800	-0.7464300

CH3a-4

40

Rh	-0.0383220	-0.8286320	-0.4012050
C	2.8845440	2.3511460	-0.2837210
C	3.6441520	1.4057690	0.3178290
H	3.1114330	3.3654930	-0.5716820
H	4.6679540	1.4319810	0.6561780
C	-2.9759820	2.2800340	0.2901190
C	-3.7831990	1.1944840	0.2668360
H	-3.2046920	3.3284820	0.3962250
H	-4.8557900	1.1136610	0.3408970
C	-1.6429450	0.4455220	0.0299540
C	1.5972250	0.4807280	-0.0521450
N	-1.6784590	1.8123550	0.1457400
N	-2.9666770	0.0889260	0.1077590
N	1.6431860	1.7692170	-0.5023640
N	2.8488520	0.2761160	0.4544450
C	3.3690160	-0.9467250	1.0640880
H	3.9025400	-0.6904890	1.9817330
H	2.5465420	-1.6115040	1.3097070
H	4.0542940	-1.4523970	0.3785930
C	-3.5321410	-1.2556240	-0.0293270
H	-3.4584310	-1.5992280	-1.0631960
H	-3.0197130	-1.9540850	0.6292940
H	-4.5837440	-1.2103830	0.2558140
C	-0.5433210	2.7383070	0.1570030
H	-0.9717410	3.7377480	0.0595540
H	-0.0365400	2.6901120	1.1256210
C	0.4778180	2.5117040	-0.9695340
H	0.8393210	3.4759630	-1.3325080
H	0.0154510	1.9952520	-1.8140710
Si	-0.1872580	-1.4961960	1.8021610
H	-1.5791270	-1.7364580	2.2710300
H	0.4296920	-0.5024580	2.7226980
H	0.5574460	-2.7833990	1.9427800
C	0.0330070	-2.8763070	-1.3992740
C	1.3214580	-2.3122770	-1.2756930
H	-0.2552100	-3.7037360	-0.7568980
H	-0.4639000	-2.8733900	-2.3668680
H	1.7906670	-1.8689650	-2.1512160
H	2.0075930	-2.7281680	-0.5467990
H	-1.1740660	-1.9157010	-0.7787940

CH4

40

Rh	0.0644300	-0.8102300	-0.3545800
C	2.7388800	2.4373400	-0.3400100

C	3.5843400	1.5098100	0.1661900
H	2.8966300	3.4720400	-0.5997400
H	4.6266800	1.5763600	0.4345100
C	-3.1466400	2.1352100	0.2674600
C	-3.8805700	0.9983000	0.2111300
H	-3.4447800	3.1634200	0.3981500
H	-4.9457800	0.8434500	0.2762800
C	-1.6926300	0.4008500	-0.0310600
C	1.5674500	0.4978200	-0.1034200
N	-1.8211800	1.7540500	0.1174400
N	-2.9871100	-0.0447000	0.0300600
N	1.5117400	1.8092300	-0.4954000
N	2.8620700	0.3350700	0.3076200
C	3.5041800	-0.8955600	0.7733100
H	3.9581100	-1.4284500	-0.0654200
H	4.2786800	-0.6290600	1.4942000
H	2.7726100	-1.5344700	1.2571600
C	-3.4262200	-1.4328900	-0.1145500
H	-4.4841400	-1.4902300	0.1431100
H	-3.2982500	-1.7725400	-1.1451800
H	-2.8686400	-2.0784700	0.5642400
C	-0.7256600	2.7226400	0.1526800
H	-1.1826300	3.7076900	0.0367700
H	-0.2380600	2.6975500	1.1323600
C	0.3181000	2.5167300	-0.9554100
H	0.6588200	3.4900600	-1.3135800
H	-0.1233900	1.9914700	-1.8050200
Si	-0.0137200	-1.1769400	1.9223900
H	-0.9742300	-2.3380900	-0.9293700
H	1.0189700	-2.1589300	2.3633100
H	-1.3427000	-1.7575900	2.2720000
H	0.1725700	0.0666500	2.7185300
C	-0.1013900	-3.0597100	-1.2138000
C	1.2334200	-2.4184400	-0.9715800
H	-0.3114400	-3.9294300	-0.5874500
H	-0.3333600	-3.2762900	-2.2597700
H	1.8090800	-2.2009500	-1.8751000
H	1.8498400	-2.9246300	-0.2310600

CH4-5

40

Rh	0.1212440	-0.8768370	-0.0224040
C	2.1821020	2.8172480	-0.5415620
C	3.1203700	1.9380420	-0.9564870
H	2.2024890	3.8937910	-0.4846850
H	4.1206200	2.0961310	-1.3265230
C	-3.4225550	1.6177100	0.3466200
C	-3.9289290	0.6433440	-0.4492230
H	-3.8918220	2.4792260	0.7950480
H	-4.9268520	0.4901180	-0.8288350
C	-1.7219980	0.1859290	-0.1421730
C	1.2927360	0.7308730	-0.3331680
N	-2.0780450	1.3188220	0.5195100
N	-2.8794440	-0.2157700	-0.7446460
N	1.0702320	2.0786960	-0.1587040
N	2.5761650	0.6753700	-0.8163950
C	3.3420270	-0.5260800	-1.1520400

H	2.8898680	-1.0481620	-1.9958650
H	4.3495330	-0.2143420	-1.4277380
H	3.3946230	-1.1906840	-0.2921490
C	-3.0334110	-1.4086360	-1.5748820
H	-3.7537650	-1.2048020	-2.3691620
H	-2.0753720	-1.6564410	-2.0321640
H	-3.3874330	-2.2558230	-0.9804090
C	-1.1132760	2.1740870	1.1990060
H	-1.6767240	2.9671590	1.6958240
H	-0.5887630	1.6049310	1.9667930
C	-0.1408660	2.8308850	0.2235860
H	0.2270970	3.7500130	0.6861420
H	-0.6791380	3.1133450	-0.6878620
Si	1.0864120	-0.8908160	2.0893890
H	-0.9421690	-2.4790830	0.2010560
H	2.5671800	-0.7362990	2.1131930
H	0.7357070	-2.1639200	2.7775780
H	0.5341180	0.2253800	2.9127290
C	-0.0994860	-3.2673700	0.0923240
C	1.2565250	-2.6302360	-0.1033930
H	-0.1962270	-3.8208700	1.0283990
H	-0.4495550	-3.8700650	-0.7489810
H	1.6506370	-2.7366910	-1.1163750
H	2.0083940	-2.9484260	0.6207500

CH4-6*

40

Rh	-0.2957320	-0.2628990	-0.6629330
C	4.0122180	-0.7035490	0.1520210
C	3.6653990	-1.9976900	-0.0759080
H	4.9706040	-0.2597760	0.3615500
H	4.2638880	-2.8965160	-0.0991570
C	-0.0326310	3.6411180	0.7307070
C	-1.1886490	3.7484100	0.0304590
H	0.5254270	4.3739960	1.2853070
H	-1.8243470	4.6005690	-0.1460220
C	-0.5102420	1.5977130	-0.1340280
C	1.7642750	-0.7575260	-0.1809150
N	0.3752480	2.3214980	0.6258710
N	-1.4728340	2.4998870	-0.4904650
N	2.8376950	0.0329730	0.0858320
N	2.2922300	-2.0107530	-0.2632340
C	1.4919820	-3.2142610	-0.4903290
H	1.4433740	-3.4632020	-1.5561570
H	1.9223210	-4.0554630	0.0567070
H	0.4917690	-3.0198250	-0.1023910
C	-2.6768200	2.2443480	-1.2931850
H	-3.2484930	3.1697530	-1.3358290
H	-2.4054090	1.9374610	-2.3010490
H	-3.2810260	1.4674070	-0.8262260
C	1.5703990	1.8074800	1.2974380
H	1.8835390	2.5898890	1.9912910
H	1.3001640	0.9309720	1.8873550
C	2.7380040	1.4693060	0.3520480
H	3.6802570	1.7699790	0.8124220
H	2.6382830	2.0177530	-0.5885580
Si	-1.5761430	-0.9779900	1.1246630

H	-4.8853340	-1.9042410	0.0526570
H	-0.6186500	-1.3612710	2.2072910
H	-2.4304960	0.1081830	1.6829830
H	-1.7702350	-0.1048280	-1.1970790
C	-4.5197740	-2.7281830	0.6856150
C	-3.0071740	-2.9565710	0.5027220
H	-4.7764320	-2.4849180	1.7263370
H	-5.0769420	-3.6290940	0.4046070
H	-2.8227130	-3.2576460	-0.5398290
H	-2.6718960	-3.7966600	1.1325960

CH6*

40

Rh	0.0991870	0.5725090	0.2545580
C	2.4845000	-2.9094790	0.2289440
C	3.4170730	-2.0485920	-0.2795880
H	2.5620250	-3.9587480	0.4871590
H	4.4554890	-2.2006870	-0.5483740
C	-3.3667620	-2.0109970	-0.3784690
C	-3.9962420	-0.8032680	-0.2357970
H	-3.7571650	-3.0172250	-0.5376780
H	-5.0483390	-0.5447560	-0.2523960
C	-1.7384400	-0.4199300	-0.0601430
C	1.4752700	-0.8563170	-0.0108520
N	-2.0026210	-1.7608750	-0.2700980
N	-2.9982070	0.1522140	-0.0413520
N	1.3098770	-2.1738220	0.3801460
N	2.7908670	-0.8125390	-0.4270580
C	3.4433670	0.3479440	-1.0412310
H	4.0740180	0.8889260	-0.3033540
H	4.0787420	0.0096660	-1.8707560
H	2.6667980	1.0185950	-1.4329820
C	-3.3730150	1.5586990	0.1386480
H	-4.4679510	1.6255570	0.1661160
H	-2.9746530	1.9551760	1.0895230
H	-3.0111910	2.1741150	-0.7076550
C	-0.9928160	-2.8248120	-0.3601540
H	-1.5454660	-3.7796310	-0.3346990
H	-0.4737960	-2.7577140	-1.3375430
C	0.0368830	-2.7821590	0.7870660
H	0.2719690	-3.8137070	1.1048650
H	-0.3712170	-2.2464540	1.6584710
Si	-0.3895940	2.8115020	-0.4951680
H	1.7197760	1.4457490	1.1005080
H	-0.7864430	2.6539680	-1.9362980
H	-1.3214660	3.8523890	0.0723140
H	-0.9104950	1.7671890	0.8188800
C	1.8996020	2.5694250	1.1097970
C	1.4128590	3.3289360	-0.1532240
H	1.3912040	2.9249570	2.0245700
H	2.9867510	2.6482050	1.2686090
H	2.0388980	3.0821630	-1.0228790
H	1.5003150	4.4167920	0.0094160

CH5

40

Rh	-0.4222730	-0.8789810	-0.1065720
C	3.5698280	0.7210230	-0.4331250
C	3.8165520	-0.1416000	0.5842820
H	4.2221650	1.4038950	-0.9545500
H	4.7261010	-0.3545280	1.1236220
C	-0.7879130	3.2881510	0.5660350
C	-1.6600710	2.8004940	1.4764810
H	-0.4931810	4.3013770	0.3438420
H	-2.2669720	3.3023530	2.2130590
C	-0.8108330	1.0290160	0.3388480
C	1.6273090	-0.3609970	0.0348400
N	-0.2676240	2.1991190	-0.1276790
N	-1.6677680	1.4230240	1.3260830
N	2.2266300	0.5715570	-0.7518730
N	2.6179030	-0.7907770	0.8604540
C	2.4746200	-1.8184590	1.8891400
H	2.8710000	-1.4519320	2.8387710
H	1.4159600	-2.0467800	2.0128050
H	3.0100210	-2.7269820	1.6004940
C	-2.5121270	0.5348350	2.1248680
H	-3.0009240	1.1299380	2.8966220
H	-3.2714870	0.0678110	1.4958130
H	-1.9064750	-0.2369560	2.6012980
C	0.6626840	2.4613590	-1.2438610
H	0.0867340	2.8675660	-2.0828410
H	1.3379330	3.2469680	-0.8921960
C	1.4852130	1.2905550	-1.7781900
H	2.1950470	1.6965050	-2.5038440
H	0.8505660	0.5732430	-2.2959590
Si	-1.9255270	-0.4509320	-1.8511360
H	-3.2809180	0.0331180	-1.4734710
H	-1.3286650	0.6335150	-2.6916670
H	-2.0713710	-1.6437520	-2.7297890
C	-0.9361490	-3.2235380	-0.2367210
C	-2.0204160	-2.2188220	0.0876570
H	-1.0939990	-3.7381690	-1.1863940
H	-0.7315070	-3.9435470	0.5590650
H	-2.3058090	-2.1839480	1.1411300
H	-2.9172260	-2.3248010	-0.5242090
H	0.0964940	-2.7302570	-0.3903610

CH5 - 6

40

Rh	-0.4678200	-0.7356000	0.0502800
C	-0.1767300	3.4777100	0.1914600
C	-0.9797800	3.2354100	1.2515000
H	0.1985500	4.4045500	-0.2126600
H	-1.4426500	3.9084400	1.9556400
C	3.5688400	0.0013500	-0.7345000
C	3.7434900	-0.7671100	0.3694400
H	4.2869100	0.4681800	-1.3902600
H	4.6441400	-1.0974000	0.8624700
C	1.5116500	-0.5954300	0.0213900
C	-0.4621600	1.2263200	0.3217100

N	2.1976100	0.0972500	-0.9323200
N	2.4771900	-1.1183600	0.8258200
N	0.1417500	2.2431500	-0.3699300
N	-1.1390900	1.8597800	1.3273400
C	-1.9486200	1.2001600	2.3495800
H	-1.4888700	0.2461600	2.6093000
H	-1.9824000	1.8351800	3.2363000
H	-2.9684900	1.0330200	1.9916700
C	2.2354100	-1.9509900	2.0014200
H	2.8169700	-1.5746900	2.8460800
H	1.1737100	-1.8990700	2.2432300
H	2.5176200	-2.9887100	1.8027100
C	1.5091000	0.8246100	-1.9912700
H	2.2025900	0.9692200	-2.8239000
H	0.6827600	0.2021000	-2.3364100
C	1.0095500	2.2003100	-1.5591800
H	0.4645200	2.6393100	-2.4025600
H	1.8657400	2.8475600	-1.3439500
Si	-2.5877300	-0.6027500	-1.5847800
H	-0.3843700	-2.7393700	-0.1181700
H	-3.8019600	0.1684900	-1.2113700
H	-2.9192900	-1.6350800	-2.5999500
H	-1.6769400	0.3519700	-2.2759600
C	-1.4764300	-3.0323400	-0.1228300
C	-2.4514500	-1.8568600	0.0103700
H	-1.6071300	-3.5595400	-1.0706500
H	-1.5639500	-3.7408000	0.7048000
H	-2.4962900	-1.4751500	1.0404000
H	-3.4803600	-2.1754400	-0.1934500

CH6

40

Rh	-0.7033700	-0.1769800	-0.1679400
C	2.0735800	2.9998700	-0.1490700
C	1.2006500	3.4329000	0.7878100
H	2.9758700	3.4483500	-0.5338300
H	1.1934400	4.3307400	1.3852700
C	3.0416500	-2.0362900	-0.2709100
C	2.6336500	-2.5810300	0.9029000
H	3.9576800	-2.1618600	-0.8265800
H	3.1262900	-3.2741300	1.5664900
C	0.9536900	-1.2543600	0.1640100
C	0.4439200	1.4238200	0.0394800
N	2.0005100	-1.2290500	-0.7091200
N	1.3585600	-2.0871200	1.1593500
N	1.6091100	1.7663400	-0.5997200
N	0.2189400	2.4601600	0.9006300
C	-0.8966200	2.5534500	1.8389600
H	-1.2460900	1.5467300	2.0649300
H	-0.5522000	3.0353800	2.7561000
H	-1.7165100	3.1388800	1.4129500
C	0.5679800	-2.4381700	2.3366800
H	1.1804000	-2.3353000	3.2352800
H	-0.2774300	-1.7527800	2.3969800
H	0.2044800	-3.4669500	2.2634900
C	1.9706500	-0.3957900	-1.9062900
H	2.6705300	-0.8061600	-2.6393400

H	0.9616300	-0.4545400	-2.3191600
C	2.3629700	1.0567400	-1.6468100
H	2.2554300	1.6057600	-2.5893200
H	3.4173100	1.1024300	-1.3560500
Si	-3.3868000	0.5488400	-0.3151000
H	-1.8269600	-1.8569900	0.2406500
H	-3.5752900	0.9004500	1.1120800
H	-4.1561200	1.4986400	-1.1553300
H	-1.9515500	0.9283200	-0.8085500
C	-2.4180600	-2.0639600	-0.6893600
C	-3.7401500	-1.2766600	-0.6865500
H	-1.8196000	-1.8420000	-1.5832200
H	-2.5516100	-3.1503900	-0.6663200
H	-4.4240500	-1.6635500	0.0772600
H	-4.2520400	-1.3862000	-1.6480200

CH6-7

40

Rh	-0.7044960	0.0782310	-0.1977080
C	2.7796690	2.4149070	-0.2011670
C	2.0227220	3.1120940	0.6747360
H	3.7776930	2.5925820	-0.5693640
H	2.2313510	4.0150920	1.2262200
C	2.3977930	-2.7433180	-0.1231910
C	1.8256280	-3.1183990	1.0497850
H	3.2563970	-3.1345370	-0.6461370
H	2.0900100	-3.9011690	1.7432610
C	0.5971610	-1.4055080	0.2260170
C	0.7941930	1.3276700	-0.0042940
N	1.6308790	-1.6958150	-0.6129340
N	0.7312150	-2.2854490	1.2526090
N	2.0257920	1.3168870	-0.6103320
N	0.8186880	2.4342010	0.7947640
C	-0.2651060	2.8762240	1.6692020
H	-0.8178620	2.0040630	2.0153680
H	0.1643260	3.4001940	2.5247740
H	-0.9427490	3.5506280	1.1384710
C	-0.1571180	-2.3636620	2.4101190
H	0.4297300	-2.3302120	3.3309870
H	-0.8289660	-1.5055380	2.3795590
H	-0.7386850	-3.2890270	2.3846390
C	1.8544550	-0.9231410	-1.8306620
H	2.4442410	-1.5253510	-2.5269800
H	0.8782210	-0.7307550	-2.2805340
C	2.6058210	0.3837070	-1.5924410
H	2.6886420	0.9009710	-2.5550850
H	3.6204550	0.1611870	-1.2472640
Si	-3.0533090	1.1337250	-0.2262690
H	-2.1467880	-1.6223540	-1.5077570
H	-3.2426270	1.8791370	1.0411120
H	-3.8084160	1.8212470	-1.3036000
H	-1.6129040	1.4068970	-0.8628970
C	-3.2350870	-1.5395330	-1.3600310
C	-3.5975570	-0.6882570	-0.1247750
H	-3.6431370	-1.1071720	-2.2786110
H	-3.6265620	-2.5571730	-1.2657600
H	-3.2163990	-1.1504480	0.7942410

H	-4.6887630	-0.6562910	0.0014510
---	------------	------------	-----------

CH7
40

Rh	0.6895330	-0.3054630	-0.0703360
C	-3.2909870	-1.7013080	-0.3978830
C	-2.7980810	-2.5594090	0.5236190
H	-4.2712860	-1.6280470	-0.8416060
H	-3.2647630	-3.3796450	1.0456520
C	-1.6477970	3.1788150	-0.2136400
C	-1.1020450	3.4113430	1.0070080
H	-2.3466060	3.7585540	-0.7961180
H	-1.2343120	4.2336490	1.6924530
C	-0.2423060	1.4582360	0.2530330
C	-1.1196810	-1.1357020	-0.0369170
N	-1.1075050	1.9803070	-0.6601310
N	-0.2493110	2.3467840	1.2802970
N	-2.2590960	-0.8277480	-0.7334070
N	-1.4771500	-2.1984630	0.7408130
C	-0.5932970	-2.8964110	1.6726580
H	0.1278230	-2.1855320	2.0754120
H	-1.1920310	-3.3102450	2.4858150
H	-0.0619510	-3.7083760	1.1678800
C	0.5312440	2.2164730	2.5088460
H	-0.1239190	2.3222570	3.3766750
H	0.9855330	1.2256180	2.5194010
H	1.3113210	2.9814640	2.5497330
C	-1.4148470	1.2769600	-1.9010510
H	-1.7599070	2.0028880	-2.6422260
H	-0.4852980	0.8297570	-2.2605820
C	-2.5006700	0.2159620	-1.7439910
H	-2.6384690	-0.2685380	-2.7172860
H	-3.4463750	0.6986060	-1.4773280
Si	2.7889250	-1.6382600	-0.1988580
H	4.0994640	1.8317690	-1.3369080
H	3.1311350	-2.3574390	1.0501280
H	3.4168850	-2.3038000	-1.3631010
H	1.2518800	-1.9128450	-0.5193300
C	3.9393270	0.7513160	-1.4042640
C	3.1953300	0.2212630	-0.1619090
H	3.3810500	0.5500500	-2.3228240
H	4.9187420	0.2744020	-1.5004220
H	3.7561600	0.4178990	0.7588000
H	2.2852710	0.8776450	-0.0211500

CH7 - GT3
40

Rh	-0.5280740	-0.2139700	-0.0746210
C	2.2093860	2.9564470	-0.2549860
C	1.3698540	3.4083920	0.7027420
H	3.0929990	3.4003030	-0.6855950
H	1.3787660	4.3217730	1.2760300
C	3.1613960	-2.1648450	-0.4506840
C	2.8043590	-2.7300880	0.7319520
H	4.0389790	-2.3050570	-1.0622080

H	3.3111890	-3.4591970	1.3444080
C	1.1300580	-1.3323140	0.1270150
C	0.6024200	1.3782530	0.0369580
N	2.1241780	-1.3156440	-0.8057260
N	1.5653250	-2.2045390	1.0753890
N	1.7386000	1.7078080	-0.6570850
N	0.3992440	2.4337880	0.8799450
C	-0.6866620	2.5501100	1.8512070
H	-0.9443650	1.5563400	2.2161790
H	-0.3474670	3.1651060	2.6865280
H	-1.5660190	3.0163340	1.3979580
C	0.8264790	-2.5605370	2.2851750
H	1.4747790	-2.4579400	3.1583580
H	-0.0178100	-1.8768190	2.3801340
H	0.4619470	-3.5893570	2.2230930
C	2.0418780	-0.4578920	-1.9834100
H	2.7016140	-0.8596770	-2.7571770
H	1.0131170	-0.4992750	-2.3468560
C	2.4636060	0.9840850	-1.7167240
H	2.3514330	1.5422490	-2.6531160
H	3.5229810	1.0078020	-1.4417090
Si	-3.1154710	0.3985320	0.0569280
H	-5.8608130	-1.8770150	-1.3589810
H	-3.0063020	-0.1272490	1.4462520
H	-3.8033400	1.7127290	0.1126800
H	-1.7736260	0.8702380	-0.6416310
C	-5.3957070	-1.1824100	-0.6530550
C	-3.9696580	-0.8147170	-1.1106150
H	-6.0381560	-0.2982060	-0.5910080
H	-5.3946820	-1.6633860	0.3305170
H	-3.3593170	-1.7233260	-1.2035540
H	-3.9918790	-0.3639680	-2.1104530

GT4-CH1

51

C	-1.97290100	1.98948100	2.21680000
C	-0.68596600	2.12440200	2.55531900
H	-2.43863200	2.64155900	1.48343500
H	-2.61153900	1.24909100	2.68964700
H	-0.05855400	2.89229100	2.11188900
H	-0.23412900	1.51007200	3.32824000
Rh	-0.19537900	-0.13659600	0.29466900
C	2.87614000	2.72538400	-0.50579400
C	2.03227100	3.14340600	-1.48227800
H	3.84834400	3.08672800	-0.20951500
H	2.12766400	3.94001000	-2.20309000
C	3.21201300	-2.41833400	-0.71186500
C	2.23292400	-3.12660400	-1.31846000
H	4.27843000	-2.57504700	-0.67636400
H	2.27790400	-4.01837300	-1.92304500
C	1.24384600	-1.37574900	-0.26433600
C	1.01877000	1.41485000	-0.41942400
N	2.60065500	-1.34634500	-0.06740400
N	1.03856500	-2.48035100	-1.04200200
N	2.23989100	1.66790500	0.12892900
N	0.90801200	2.32819200	-1.42123900
C	-0.24370200	2.47890000	-2.31016300

H	0.08023300	2.97674300	-3.22501500
H	-0.63798800	1.49585000	-2.56501400
H	-1.02626700	3.07550500	-1.83501400
C	-0.25967600	-2.95238700	-1.52423900
H	-0.08711200	-3.69021200	-2.30879000
H	-0.82428100	-3.41542600	-0.71167400
H	-0.83130100	-2.11830700	-1.93054000
C	3.43151500	-0.43772200	0.74251900
H	3.77149000	-0.98098200	1.63147900
H	4.31391200	-0.20537400	0.13799200
C	2.78344200	0.86100400	1.21449200
H	3.55342800	1.44285300	1.72863800
H	1.97950800	0.65924700	1.92088600
Si	-3.26981500	0.41822400	-1.07863900
H	-1.95685900	0.70705700	-0.36819200
H	-6.34547100	0.22608800	-0.95889300
H	-3.74877800	1.74597700	-1.54989100
H	-2.92640000	-0.40908100	-2.26610100
C	-4.51290900	-0.42902800	0.05700600
C	-5.86933300	-0.70065200	-0.62284900
H	-4.65423500	0.20039200	0.94448300
H	-4.07077500	-1.36675400	0.41560900
H	-5.76085800	-1.35407300	-1.49464300
H	-6.55975200	-1.19058800	0.07047300
Si	-0.30012900	-1.47518700	2.26189000
H	-1.50481200	-1.25873700	3.10711800
H	-1.19324500	-1.37104000	0.70476300
H	-0.08862900	-2.94148600	2.12289800
H	0.87149800	-0.97717000	3.05428400

CH2-mCH3

40

Rh	-0.4956100	-0.8046790	-0.0748430
C	3.5930780	0.0474710	-0.5216510
C	3.7003000	-0.7667110	0.5552570
H	4.3467750	0.5711380	-1.0883600
H	4.5641290	-1.0858060	1.1166710
C	-0.0367110	3.5758640	0.1679820
C	-0.9100710	3.3558580	1.1766800
H	0.4221120	4.4874280	-0.1818070
H	-1.3522950	4.0342370	1.8893800
C	-0.5066360	1.3443850	0.1783250
C	1.5047960	-0.6698580	0.0060570
N	0.2100690	2.3414290	-0.4272750
N	-1.1800870	1.9956870	1.1739050
N	2.2423160	0.1013170	-0.8466220
N	2.4149390	-1.2010420	0.8642480
C	2.1156170	-2.0809070	1.9917770
H	2.1884430	-1.5327630	2.9353580
H	1.1082580	-2.4744080	1.8716850
H	2.8224880	-2.9130900	2.0033700
C	-1.9953130	1.3608120	2.2062190
H	-1.4923970	1.4218560	3.1754810
H	-2.9688310	1.8518250	2.2719150
H	-2.1512610	0.3138870	1.9477480
C	1.1617510	2.2663620	-1.5469460
H	0.7008920	2.7103400	-2.4367730

H	2.0117180	2.8975080	-1.2691800
C	1.6736280	0.8812270	-1.9424060
H	2.4551210	1.0289830	-2.6926540
H	0.8849760	0.2919400	-2.4080520
Si	-3.0972170	-0.6076740	-0.9688760
H	-2.6882630	-0.2259880	-2.3423900
H	-3.3080080	0.5979440	-0.1304320
H	-4.4379090	-1.2391740	-1.0518350
C	-0.8101150	-2.8291100	-0.1509110
C	-2.2299910	-2.4132010	-0.3657830
H	-0.3621450	-3.3945810	-0.9663870
H	-0.6297020	-3.3216270	0.8084040
H	-2.9054720	-2.6556060	0.4572650
H	-2.6273480	-2.8273880	-1.2984390
H	-0.2904530	-0.9135340	-1.5561520

CH3-3a

40

Rh	-0.0900210	-0.8173090	-0.4477290
C	2.9352850	2.3167770	-0.1601560
C	3.6462200	1.3955690	0.5305680
H	3.1865370	3.3172780	-0.4751710
H	4.6451760	1.4315720	0.9358960
C	-2.8829140	2.3809710	0.3407930
C	-3.7234550	1.3231050	0.3679180
H	-3.0723370	3.4372120	0.4458680
H	-4.7929730	1.2780830	0.4952910
C	-1.6231790	0.5029490	0.0327030
C	1.6193280	0.4606890	0.0683070
N	-1.6093280	1.8722520	0.1330690
N	-2.9544590	0.1901250	0.1739040
N	1.7085900	1.7272980	-0.4358080
N	2.8350940	0.2758850	0.6630500
C	3.3215940	-0.9233000	1.3451180
H	2.4855100	-1.5722920	1.5826420
H	4.0414850	-1.4537720	0.7158130
H	3.8113820	-0.6296920	2.2760240
C	-3.5881430	-1.1287040	0.0750200
H	-4.6525650	-1.0019430	0.2739890
H	-3.4581700	-1.5425790	-0.9255310
H	-3.1789250	-1.8186540	0.8119290
C	-0.4658740	2.7882120	0.0748310
H	-0.8876240	3.7745300	-0.1291700
H	0.0207300	2.8339320	1.0543160
C	0.5789770	2.4569750	-0.9982480
H	0.9726440	3.3847510	-1.4186190
H	0.1319240	1.8911900	-1.8196710
Si	-0.4971150	-1.9470380	1.5301920
H	-0.9890170	-3.3291620	1.2703320
H	-1.4976450	-1.2624700	2.3919440
H	0.7488760	-2.0719200	2.3342900
C	0.3825290	-2.6706780	-1.6801550
C	1.5878140	-2.1298050	-1.2762410
H	-0.0324110	-3.5443230	-1.1892670
H	-0.0206680	-2.4578960	-2.6666320
H	2.1595800	-1.4936180	-1.9453640
H	2.1432550	-2.5780800	-0.4613210

H	-1.3425940	-1.6502120	-0.8947110
---	------------	------------	------------

CH3a - mCH4a

40

Rh	0.5799190	-0.6229880	0.3407130
C	-0.0056180	3.5503950	-0.4327150
C	0.5969600	3.6734510	0.7762680
H	-0.3836230	4.2976830	-1.1128330
H	0.8372840	4.5498760	1.3573400
C	-3.7132880	-0.2926310	-0.5680800
C	-3.6955580	-1.2955930	0.3392580
H	-4.5347280	0.1814110	-1.0819440
H	-4.5001720	-1.8667400	0.7744650
C	-1.5319890	-0.6653740	-0.0093860
C	0.5130370	1.4585300	0.2975980
N	-2.3906500	0.0867680	-0.7689930
N	-2.3686080	-1.5072130	0.6714950
N	-0.0482130	2.1890470	-0.7084090
N	0.9085240	2.3894240	1.2055890
C	1.5469510	2.0996850	2.4890210
H	2.3825750	2.7855630	2.6437790
H	0.8285710	2.2135680	3.3052060
H	1.9124840	1.0738200	2.4669710
C	-1.9541140	-2.5232460	1.6407370
H	-1.2357420	-2.1011060	2.3429580
H	-2.8358840	-2.8562480	2.1896860
H	-1.5039230	-3.3794390	1.1326780
C	-2.1129620	1.1859120	-1.7061290
H	-2.5001330	0.8922280	-2.6881630
H	-2.6878200	2.0569790	-1.3732970
C	-0.6542390	1.5818620	-1.8884620
H	-0.6096500	2.3074670	-2.7052560
H	-0.0588300	0.7151280	-2.1714540
Si	2.0910520	-2.2786730	-0.1347090
H	2.1058090	-0.4798610	0.8545310
H	3.0859100	-2.7268040	0.8685870
H	1.7204430	-3.4386830	-0.9876420
H	0.4622110	-2.2551750	0.5173140
C	2.2668790	-0.6699690	-1.8802920
C	3.3842610	-1.4642400	-1.5775430
H	1.5321660	-1.0163070	-2.6016090
H	2.2314960	0.3725920	-1.5996710
H	4.2214730	-1.0018230	-1.0601270
H	3.6097230	-2.3271140	-2.1971230

CH3a - mCH4b

40

Rh	0.7221200	-0.4635600	-0.3859700
C	-3.3320100	-1.1677700	0.8452900
C	-3.3841400	-1.8465300	-0.3274700
H	-4.0844600	-1.0035600	1.6006800
H	-4.1945200	-2.3829100	-0.7955700
C	-0.9858700	3.5007800	0.3375300
C	-0.1793400	3.7446400	-0.7207800
H	-1.6507200	4.1514300	0.8837300

H	-0.0155400	4.6461500	-1.2896600
C	0.0964300	1.5549600	-0.1564200
C	-1.2715900	-1.0457400	-0.1155300
N	-0.8146800	2.1620900	0.6714400
N	0.4717200	2.5573200	-1.0079700
N	-2.0339000	-0.6841200	0.9552600
N	-2.1205700	-1.7607100	-0.9002400
C	-1.7784100	-2.3633000	-2.1871700
H	-2.3484200	-1.8879300	-2.9896400
H	-0.7140700	-2.2174200	-2.3648200
H	-2.0009800	-3.4329100	-2.1684800
C	1.3711400	2.4225100	-2.1551000
H	0.8160300	2.1076500	-3.0426700
H	1.8407800	3.3886400	-2.3473100
H	2.1335600	1.6791000	-1.9285000
C	-1.5729300	1.6234700	1.8133700
H	-1.2159000	2.1169800	2.7247900
H	-2.6166800	1.9210400	1.6693000
C	-1.5090700	0.1187600	2.0499500
H	-2.0975700	-0.0931400	2.9470600
H	-0.4865200	-0.2045000	2.2374700
Si	2.5609900	-1.7702700	-0.0112800
H	1.0067400	-2.0032400	-0.8529900
H	3.7139700	-1.8061500	-0.9425200
H	2.4177000	-3.1152400	0.6055600
H	2.2251800	0.0964800	-0.6811000
C	2.1915400	-0.5275600	1.9843200
C	3.4979500	-0.9390400	1.6819100
H	1.5398300	-1.1812900	2.5568600
H	1.8838200	0.5020500	1.8684100
H	4.2096800	-0.1937200	1.3349200
H	3.9084700	-1.8166600	2.1724700

mCH3

40

Rh	-0.7652560	-0.0469030	-0.0840880
C	2.5017670	-2.6671910	-0.2804670
C	1.8678960	-3.2430580	0.7688090
H	3.4202980	-2.9294020	-0.7812430
H	2.1253490	-4.1056010	1.3628930
C	2.6623780	2.7573290	-0.0353880
C	1.7761430	3.4291820	0.7347010
H	3.6638460	3.0122250	-0.3449440
H	1.8505030	4.3869600	1.2251950
C	0.7836200	1.4717170	0.1102960
C	0.6098390	-1.4795090	0.1120270
N	2.0482030	1.5651780	-0.4066950
N	0.6448030	2.6331910	0.8180410
N	1.7199200	-1.5856110	-0.6704570
N	0.7134300	-2.5031510	1.0007260
C	-0.2478270	-2.8316280	2.0535110
H	0.2946880	-3.1945220	2.9281610
H	-0.8040730	-1.9374630	2.3299800
H	-0.9471230	-3.5986520	1.7131270
C	-0.5533170	3.0391410	1.5503020
H	-1.0366450	2.1651110	1.9870050
H	-0.2634980	3.7134510	2.3576420

H	-1.2592370	3.5526770	0.8918420
C	2.8151410	0.5999940	-1.2125860
H	3.1926230	1.1376910	-2.0887910
H	3.6826380	0.2860620	-0.6211250
C	2.0800140	-0.6355620	-1.7198270
H	2.7509000	-1.1495630	-2.4131670
H	1.1795230	-0.3628770	-2.2693670
Si	-3.3801250	0.9617180	-0.5181300
H	-0.6922710	-0.2663980	-1.5721760
H	-3.8286100	2.0137950	-1.4632910
H	-3.8881680	1.2460720	0.8476140
H	-1.8667580	1.3465480	-0.4165540
C	-2.3321820	-1.4612240	-0.2299070
C	-3.5008810	-0.8396370	-1.0258770
H	-2.6502720	-1.6484440	0.8080480
H	-2.0249200	-2.4223310	-0.6539090
H	-3.3201490	-0.9102720	-2.1042300
H	-4.4804230	-1.2930830	-0.8297830

mCH3 - CH6

40

Rh	-0.7578960	-0.1586110	-0.2125130
C	2.8628800	-2.2415990	-0.2881570
C	2.3601610	-2.8493130	0.8139950
H	3.7989150	-2.3794480	-0.8061030
H	2.7726440	-3.6208900	1.4446130
C	2.3353900	2.9374640	0.0242060
C	1.4278460	3.4386340	0.8940200
H	3.2946350	3.3170990	-0.2912710
H	1.4422780	4.3374960	1.4901910
C	0.5850560	1.4853520	0.0868710
C	0.8081430	-1.3622350	0.1069470
N	1.8133050	1.7408700	-0.4569160
N	0.3726470	2.5401400	0.9239540
N	1.8989860	-1.3333270	-0.7085360
N	1.1038410	-2.2967000	1.0469400
C	0.2355150	-2.7060520	2.1496300
H	0.8512160	-2.9386700	3.0202110
H	-0.4354740	-1.8853550	2.3977430
H	-0.3510740	-3.5865110	1.8754280
C	-0.8187760	2.7386300	1.7467920
H	-1.3371560	1.7875480	1.8620440
H	-0.5229600	3.1014180	2.7332750
H	-1.4921840	3.4648620	1.2829000
C	2.5858290	0.9589030	-1.4376930
H	2.6768190	1.5542790	-2.3530490
H	3.5920900	0.8317190	-1.0249420
C	2.0184320	-0.4027430	-1.8276660
H	2.6913220	-0.8405540	-2.5700430
H	1.0300680	-0.2993420	-2.2785800
Si	-3.4321430	0.6953460	-0.5245700
H	-1.1417520	-1.1365680	-1.3381710
H	-4.0924030	1.5306200	-1.5562700
H	-3.7630410	1.2057530	0.8288940
H	-1.9432050	1.0844170	-0.7825670
C	-2.2741450	-1.7013970	-0.1014310
C	-3.5841900	-1.1724190	-0.7071070

H	-2.3193970	-1.7055880	0.9953200
H	-2.0389420	-2.7182020	-0.4264120
H	-3.6521340	-1.4156960	-1.7733530
H	-4.4792400	-1.5819830	-0.2233380

mCH4a
40

Rh	0.1946810	-0.8053140	-0.2321900
C	-3.5135930	1.1150800	0.3687520
C	-3.8616980	0.2793970	-0.6399490
H	-4.0925460	1.8410690	0.9173240
H	-4.8046610	0.1366210	-1.1432720
C	1.6290870	3.4098460	0.0998100
C	2.6400050	2.8489780	-0.6020410
H	1.4813030	4.4237990	0.4367940
H	3.5513260	3.2759840	-0.9896990
C	1.1142120	1.2010300	-0.1817660
C	-1.6728910	-0.0868220	-0.1931690
N	0.7069570	2.3998570	0.3464040
N	2.3132230	1.5138110	-0.7677100
N	-2.1687440	0.8788230	0.6295210
N	-2.7274670	-0.4473060	-0.9744320
C	-2.7099130	-1.4963880	-1.9961810
H	-3.5966870	-1.3857030	-2.6213030
H	-1.8204940	-1.3977150	-2.6178040
H	-2.7101450	-2.4826270	-1.5276300
C	3.1918210	0.5899150	-1.4880230
H	2.6139190	-0.0164740	-2.1851600
H	3.9153690	1.1757170	-2.0559830
H	3.7287310	-0.0602130	-0.7939480
C	-0.5616130	2.7598860	1.0003800
H	-0.3064390	3.4507910	1.8095830
H	-1.1793280	3.3103240	0.2816660
C	-1.3793880	1.6252190	1.6056520
H	-2.0845710	2.0690360	2.3127000
H	-0.7460970	0.9377480	2.1624560
Si	1.9235690	-2.8281170	0.2903520
H	-0.5053150	-2.2200330	-0.4111040
H	1.6258180	-3.9474900	-0.6260060
H	3.3899780	-2.7606050	0.5343120
H	1.8280390	-1.4755480	-0.4962020
C	0.1766630	-1.3750080	1.7738560
C	0.8813010	-2.7230690	1.8715520
H	0.7419840	-0.5879920	2.2807290
H	-0.8548850	-1.4000850	2.1279260
H	0.1634490	-3.5487400	1.8649930
H	1.4989330	-2.8097430	2.7735390

mCH4b
40

Rh	0.0270200	0.8050400	-0.2476700
C	2.4375900	-2.7638500	0.4463500
C	3.1887000	-2.2205400	-0.5429300
H	2.5773500	-3.6614900	1.0279800
H	4.1132000	-2.5514100	-0.9893300

C	-3.2628200	-1.9356800	0.0625700
C	-3.8493000	-0.8850600	-0.5535500
H	-3.6637500	-2.8906400	0.3629400
H	-4.8646600	-0.7410100	-0.8864200
C	-1.6700700	-0.3300200	-0.2051800
C	1.3985900	-0.8522300	-0.2307700
N	-1.9325100	-1.5922500	0.2697900
N	-2.8751700	0.0839800	-0.7101000
N	1.3514900	-1.9145500	0.6208700
N	2.5387300	-1.0622900	-0.9474000
C	3.0622000	-0.1745600	-1.9852600
H	3.5896900	-0.7701600	-2.7321800
H	2.2363400	0.3443600	-2.4703700
H	3.7515300	0.5587300	-1.5576300
C	-3.1757800	1.3732100	-1.3434300
H	-2.4504200	1.5932200	-2.1249800
H	-4.1698400	1.3029600	-1.7868300
H	-3.1601100	2.1761900	-0.6055700
C	-1.0282000	-2.6367000	0.7833100
H	-1.6284700	-3.2253200	1.4821600
H	-0.7481800	-3.2959700	-0.0458600
C	0.2319700	-2.1867100	1.5165400
H	0.5410100	-3.0014600	2.1755300
H	0.0328800	-1.3164600	2.1406300
Si	1.2836500	3.1083900	0.2969100
H	1.4450100	1.8016900	-0.5759800
H	0.6993800	4.1870500	-0.5255500
H	2.7450200	3.3394100	0.4526500
H	-0.9688500	2.0456300	-0.2823200
C	0.0430900	1.2328500	1.7959900
C	0.4081400	2.7049500	1.9336900
H	0.8223900	0.5905100	2.2128500
H	-0.9332100	0.9753700	2.2093100
H	-0.4841400	3.3334300	2.0096300
H	1.0484200	2.9029000	2.8016300

mCH4b - 5b

40

Rh	0.3016360	-0.8131720	-0.2362840
C	-3.6034350	0.5984840	0.4403190
C	-3.8587880	-0.2183610	-0.6095180
H	-4.2603930	1.2180390	1.0302250
H	-4.7815100	-0.4419460	-1.1209810
C	0.9864600	3.6185450	0.0929140
C	2.0292640	3.2458810	-0.6841080
H	0.6762970	4.5917410	0.4398860
H	2.8083140	3.8310930	-1.1463960
C	0.8841700	1.3462820	-0.1346220
C	-1.6404720	-0.3654090	-0.1738680
N	0.2969860	2.4569970	0.4146090
N	1.9525970	1.8702440	-0.8161760
N	-2.2407210	0.4995580	0.6948390
N	-2.6533940	-0.8042320	-0.9729110
C	-2.5290420	-1.7214100	-2.1066980
H	-2.4271640	-1.1617400	-3.0405280
H	-1.6498680	-2.3465740	-1.9589120
H	-3.4213000	-2.3478840	-2.1560740

C	2.9289690	1.1185650	-1.6088330
H	2.4219070	0.4379690	-2.2928660
H	3.5129680	1.8278680	-2.1960650
H	3.6049010	0.5546140	-0.9631760
C	-0.9352600	2.5729000	1.2096790
H	-0.6956200	3.1889510	2.0825100
H	-1.6759240	3.1188520	0.6147290
C	-1.5439910	1.2743090	1.7180870
H	-2.2783640	1.5324340	2.4853060
H	-0.7844110	0.6518910	2.1853970
Si	2.5120420	-2.3910830	0.2705530
H	-0.1211440	-2.2662730	-0.6387990
H	3.9622510	-2.0695400	0.3023730
H	2.2876160	-3.6749940	-0.4236370
H	2.0173170	-1.2375030	-0.6431710
C	0.2047130	-1.8115820	1.6096770
C	1.6413500	-2.1928960	1.9388990
H	-0.4506110	-2.6780290	1.5365760
H	-0.2209910	-1.1065040	2.3257280
H	2.1515120	-1.3954380	2.4892040
H	1.7100890	-3.1089460	2.5396360

mCH4a - CH6

40

Rh	-0.5474510	-0.6672050	0.2419730
C	3.5439190	-0.2853410	-0.5708630
C	3.6604610	-0.9643170	0.5959930
H	4.2945040	0.0783350	-1.2549560
H	4.5340720	-1.2985270	1.1329370
C	0.0852200	3.7219210	-0.3571040
C	-0.8643560	3.7279970	0.6085510
H	0.6034830	4.5339200	-0.8428950
H	-1.3312640	4.5464840	1.1335210
C	-0.4581060	1.5524640	0.0755590
C	1.4486110	-0.7028860	0.1983850
N	0.3284280	2.3893360	-0.6664010
N	-1.1793030	2.4036460	0.8615390
N	2.1817100	-0.1318730	-0.8005050
N	2.3713420	-1.2158060	1.0536660
C	2.0925840	-1.9020600	2.3151490
H	2.7087860	-2.8009920	2.3827530
H	2.3146560	-1.2445590	3.1599440
H	1.0397050	-2.1771370	2.3365560
C	-2.1821510	2.0057800	1.8517990
H	-1.9101950	1.0424480	2.2812820
H	-2.2079380	2.7514960	2.6479870
H	-3.1725290	1.9371340	1.3936280
C	1.3343110	2.0550250	-1.6872660
H	1.0116780	2.4971000	-2.6363520
H	2.2709420	2.5429870	-1.3974930
C	1.5864780	0.5715750	-1.9331370
H	2.2731180	0.4918670	-2.7802670
H	0.6637180	0.0602060	-2.2066530
Si	-3.1265460	-1.3311230	-0.5584680
H	-0.5618500	-2.0021420	1.0235890
H	-4.3549060	-1.6428720	0.2111740
H	-3.4291150	-0.3520370	-1.6295660

H	-2.3250700	-0.5653630	0.5355310
C	-0.6508660	-2.3115600	-1.0737050
C	-2.0942290	-2.8184600	-1.0894700
H	-0.3844400	-1.8338450	-2.0240450
H	0.0778730	-3.0949050	-0.8621850
H	-2.2385640	-3.6124900	-0.3488910
H	-2.3962180	-3.2151030	-2.0672420

mCH5b

40

Rh	-0.7930890	0.0022100	-0.0718100
C	2.3330030	-2.7221300	-0.3596000
C	1.7921610	-3.2355690	0.7720430
H	3.1838870	-3.0370580	-0.9430390
H	2.0885190	-4.0804310	1.3732770
C	2.8463110	2.5032160	-0.1583360
C	2.0999350	3.2034140	0.7270910
H	3.8440740	2.6728470	-0.5317900
H	2.3208550	4.1036260	1.2787410
C	0.8466330	1.4249970	0.0545250
C	0.5105530	-1.4760350	0.1687800
N	2.0713400	1.4191340	-0.5595660
N	0.8921900	2.5334610	0.8471300
N	1.5338770	-1.6420380	-0.7163900
N	0.6743720	-2.4657800	1.0812420
C	-0.1577970	-2.6995250	2.2616760
H	0.3156010	-2.2746730	3.1509240
H	-1.1285440	-2.2342770	2.1077730
H	-0.2894310	-3.7741980	2.3992870
C	-0.1953480	3.0037810	1.7046190
H	-0.7612550	2.1488820	2.0707140
H	0.2296040	3.5430450	2.5527570
H	-0.8614060	3.6727630	1.1524730
C	2.6047460	0.4683300	-1.5446370
H	2.7696190	1.0043350	-2.4862360
H	3.5820820	0.1310910	-1.1833610
C	1.7401240	-0.7506510	-1.8532660
H	2.2364890	-1.3157250	-2.6468180
H	0.7616900	-0.4562170	-2.2453210
Si	-3.3670410	1.0976200	-0.4351250
H	-1.1184120	-0.0979520	1.3951620
H	-3.7943820	2.2500730	-1.2684020
H	-3.9355950	1.2017700	0.9277390
H	-1.8562680	1.4631910	-0.2610430
C	-2.3882800	-1.3729230	-0.3386480
C	-3.4498090	-0.6270020	-1.1767190
H	-2.8288860	-1.7096340	0.6054770
H	-2.0143380	-2.2651180	-0.8565560
H	-3.1606550	-0.5711910	-2.2333560
H	-4.4515100	-1.0741660	-1.1472770

mCH5b - CH6

40

Rh	-0.7321010	-0.4280020	0.1904770
C	3.2728280	-1.2721610	-0.6538380

C	3.2386970	-1.8838120	0.5552140
H	4.0719220	-1.1682360	-1.3710060
H	4.0049220	-2.4137240	1.0986950
C	1.1691470	3.4719450	-0.4145590
C	0.3589390	3.7484640	0.6343140
H	1.8671320	4.0948480	-0.9517080
H	0.2169790	4.6588070	1.1951800
C	0.0268720	1.5679410	0.0853210
C	1.1711750	-1.0440200	0.1797860
N	0.9614450	2.1350390	-0.7373330
N	-0.3253480	2.5801970	0.9271000
N	1.9974720	-0.7633060	-0.8688380
N	1.9478950	-1.7339400	1.0541450
C	1.5219140	-2.2709460	2.3460710
H	0.5447000	-1.8582930	2.5888670
H	1.4601770	-3.3615480	2.3026050
H	2.2389870	-1.9791170	3.1165400
C	-1.2987560	2.4753040	2.0148110
H	-1.3543040	1.4368720	2.3390410
H	-0.9698630	3.0977180	2.8490580
H	-2.2856180	2.8101580	1.6831760
C	1.7147460	1.5256640	-1.8448760
H	1.4036670	2.0047810	-2.7800290
H	2.7712760	1.7655580	-1.6869720
C	1.5577170	0.0178530	-2.0200980
H	2.1513390	-0.2788110	-2.8890420
H	0.5173810	-0.2470010	-2.2231730
Si	-3.3869470	-0.3915320	-0.5571820
H	-1.1066600	-1.5675890	1.1615720
H	-3.8249490	0.6872930	-1.4744350
H	-4.4590290	-0.7282410	0.4086390
H	-2.3622090	0.3002150	0.3966560
C	-1.5376450	-2.3789480	-0.3443940
C	-2.5991180	-1.9175990	-1.3533360
H	-1.9885060	-3.0404510	0.3998120
H	-0.6952930	-2.9109050	-0.7908120
H	-2.1469560	-1.6280630	-2.3068670
H	-3.3426160	-2.6968030	-1.5687180

CH4-SBM5

45

Rh	0.1648190	-0.4617710	0.2737240
C	-3.8595880	0.6410170	0.2106670
C	-4.0102530	-0.5887310	-0.3329870
H	-4.5856720	1.3974190	0.4630950
H	-4.8949210	-1.1154960	-0.6539490
C	1.1419540	3.7990700	-0.1115560
C	2.4000460	3.2995330	-0.0886890
H	0.7858580	4.8159660	-0.1574670
H	3.3571110	3.7961260	-0.1053690
C	0.9700440	1.5266580	-0.0086810
C	-1.7928440	-0.2916890	0.0428780
N	0.2841630	2.7085100	-0.0604090
N	2.2793540	1.9202110	-0.0258150
N	-2.4997960	0.8115690	0.4361510
N	-2.7450240	-1.1509970	-0.4301700
C	-2.5492890	-2.4948310	-0.9788390

H	-3.1298870	-3.2130960	-0.3951210
H	-2.8812600	-2.5175430	-2.0192820
H	-1.4960700	-2.7490370	-0.9294080
C	3.4367520	1.0280480	0.0170350
H	3.4355700	0.3637790	-0.8476240
H	4.3426160	1.6341960	-0.0029250
H	3.4307160	0.4378890	0.9354670
C	-1.1700510	2.8627680	-0.1064200
H	-1.3693590	3.9251760	0.0480710
H	-1.5372290	2.5995230	-1.1031000
C	-1.9241850	2.0486670	0.9594220
H	-2.7603530	2.6397050	1.3382740
H	-1.2701390	1.8227990	1.8042930
Si	0.2304290	-0.4639410	-2.0469880
H	-0.1912490	-1.6632350	3.3352460
H	-0.3047750	-1.7066110	-2.6721050
H	1.6619550	-0.3492500	-2.4551630
H	-0.5028720	0.6751890	-2.6713200
C	0.4810510	-1.7781230	2.4812990
C	-0.2341820	-2.2768210	1.2263590
H	0.9384600	-0.7561890	2.3442650
H	1.3315650	-2.4010960	2.7718300
H	-1.2722620	-2.5442360	1.4216440
H	0.2664780	-3.1188150	0.7425280
Si	3.1952580	-2.8605920	-0.2324150
H	4.4655390	-2.3122710	-0.7650360
H	2.5337540	-3.7376780	-1.2248030
H	3.4231650	-3.5758780	1.0453690
H	2.2791700	-1.7026450	0.0454070

SBM5

45

Rh	0.0262420	-0.7083790	0.2943490
C	-2.8811460	2.4880550	0.0948550
C	-3.6247480	1.5154200	-0.4841720
H	-3.1201880	3.5100900	0.3430210
H	-4.6408190	1.5242430	-0.8460330
C	3.0304790	2.4476200	-0.0803480
C	3.8334360	1.3580940	-0.0754120
H	3.2669000	3.4993940	-0.1066980
H	4.9083960	1.2752380	-0.0893090
C	1.6863380	0.6089150	-0.0205430
C	-1.5871440	0.6202110	-0.0336720
N	1.7256880	1.9782840	-0.0489790
N	3.0069020	0.2491400	-0.0417330
N	-1.6414290	1.9229440	0.3646280
N	-2.8248930	0.3839870	-0.5557540
C	-3.3109410	-0.8655170	-1.1474870
H	-4.2220880	-1.1814950	-0.6338840
H	-3.5280830	-0.7108750	-2.2069210
H	-2.5496580	-1.6331990	-1.0438080
C	3.5543810	-1.1109480	-0.0290230
H	3.0633550	-1.7230760	-0.7841110
H	4.6171090	-1.0482770	-0.2640950
H	3.4340270	-1.5672230	0.9553800
C	0.5921210	2.9033000	-0.1379650
H	1.0105390	3.9020480	-0.0006090

H	0.1648340	2.8595470	-1.1441810
C	-0.5117600	2.6728430	0.9050120
H	-0.9033630	3.6370220	1.2349900
H	-0.1125190	2.1624720	1.7842620
Si	0.2006940	-0.6106020	-2.0659220
H	-1.4958880	-0.3986140	3.2219190
H	-0.7968160	-1.4825250	-2.7457700
H	1.5489740	-1.0215630	-2.5379370
H	-0.0361230	0.7774810	-2.5523980
C	-0.7711250	-1.0308510	2.7014970
C	-1.3813260	-1.7693310	1.5142500
H	0.0504270	-0.3168120	2.4037550
H	-0.2872500	-1.7045920	3.4121910
H	-2.4118700	-1.4929700	1.3094150
H	-1.3354300	-2.8511230	1.6385300
Si	0.2662710	-3.1167690	-0.1802680
H	1.3100780	-3.3595090	-1.2132220
H	-1.0252020	-3.5452720	-0.7796430
H	0.5483860	-4.0099520	0.9715400
H	1.1886060	-1.8075370	0.6054920

SBM5-6

45

Rh	-0.0334720	-0.6500760	-0.1622860
C	2.5291850	2.9021370	-0.3198960
C	3.4045510	2.0764620	0.3018950
H	2.6362970	3.9194000	-0.6622620
H	4.4266440	2.2328490	0.6093230
C	-3.3466280	2.0109690	-0.0254540
C	-4.0013000	0.8268660	-0.0176540
H	-3.7176680	3.0233330	-0.0297550
H	-5.0566390	0.6069540	-0.0211480
C	-1.7777400	0.3633430	-0.0190180
C	1.4607840	0.9188250	0.0412070
N	-1.9914810	1.7185000	-0.0219540
N	-3.0414350	-0.1693780	-0.0098160
N	1.3539250	2.1784150	-0.4712460
N	2.7399970	0.8764660	0.5178180
C	3.3887870	-0.2504970	1.1896810
H	4.2171460	-0.6257060	0.5829130
H	3.7722240	0.0741340	2.1595810
H	2.6632790	-1.0428700	1.3484020
C	-3.4199680	-1.5875470	0.0001990
H	-2.9003560	-2.1115450	0.8010550
H	-4.4948770	-1.6419880	0.1757430
H	-3.1857530	-2.0554690	-0.9567150
C	-0.9900550	2.7826380	0.0791600
H	-1.5431060	3.7194260	-0.0078980
H	-0.5372440	2.7564000	1.0743280
C	0.1119670	2.7389100	-0.9924290
H	0.3361060	3.7540820	-1.3257830
H	-0.2210270	2.1713940	-1.8652610
Si	-0.3211960	-0.5931520	2.1572310
H	1.3990290	-0.9410100	-3.3663800
H	0.9005220	-1.0915640	2.8469840
H	-1.4709190	-1.4221980	2.6088660
H	-0.5570220	0.7942280	2.6541210

C	0.7348510	-1.3361880	-2.5901980
C	1.5637420	-1.8855910	-1.4189920
H	0.0601540	-0.4894540	-2.3374360
H	0.1018760	-2.1119360	-3.0255260
H	2.4230880	-1.2644800	-1.1725140
H	2.0013860	-2.8319120	-1.7573220
Si	0.8464330	-3.1830460	0.0526230
H	0.1425130	-3.2038760	1.3603330
H	2.2194460	-3.6524230	0.3966690
H	0.1802150	-4.1632740	-0.8362980
H	-1.0184910	-1.8722780	-0.3637210

SBM5-6s

45

Rh	0.1434820	-0.7149160	0.0963460
C	-3.5423400	1.6518880	0.0530180
C	-4.0182050	0.4518180	-0.3593900
H	-4.0477380	2.5838660	0.2515280
H	-5.0203890	0.1350520	-0.6018600
C	2.2606360	2.9128910	0.0507690
C	3.2969580	2.0745420	0.2651740
H	2.2163890	3.9898790	0.0318560
H	4.3347770	2.2753670	0.4765230
C	1.4574520	0.7852960	-0.0935460
C	-1.7742900	0.2306880	-0.0932150
N	1.1414200	2.1243720	-0.1816960
N	2.8048160	0.7827550	0.1637220
N	-2.1700310	1.4947600	0.2095620
N	-2.9278240	-0.4044220	-0.4423210
C	-3.0322770	-1.7842200	-0.9172170
H	-3.8616440	-2.2850100	-0.4133520
H	-3.1971470	-1.8030880	-1.9975390
H	-2.1062420	-2.3133930	-0.6941290
C	3.6822300	-0.3734590	0.3424910
H	3.6753140	-0.9989420	-0.5500910
H	4.6965530	-0.0050890	0.4958470
H	3.3865520	-0.9542980	1.2169030
C	-0.1476510	2.7417410	-0.5050050
H	0.0612230	3.8052400	-0.6309840
H	-0.4998120	2.3625950	-1.4655390
C	-1.2431230	2.5648740	0.5612910
H	-1.8291900	3.4831960	0.6340790
H	-0.8004510	2.3727920	1.5428340
Si	0.5059680	-0.4746520	-2.2756860
H	-1.2917580	-0.9766520	4.0166770
H	-0.2256770	-1.6503500	-2.8334280
H	1.9102750	-0.5281190	-2.7593870
H	-0.1031840	0.7466770	-2.8761510
C	-0.8004860	-0.5571630	3.1292180
C	-0.6523010	-1.6292770	2.0508410
H	-1.4046870	0.2890420	2.7897890
H	0.1696730	-0.1678180	3.4540400
H	-1.6193740	-1.9697070	1.6710070
H	-0.1607170	-2.5146810	2.4637530
Si	1.5250320	-2.7273200	-0.1612970
H	2.3732430	-2.7083750	-1.3812450
H	0.3677870	-3.6450640	-0.3616390

H	2.3641330	-3.2988940	0.9276550
H	0.8630980	-1.6253950	1.2235980

SBM6

45

Rh	0.0309850	0.5644030	0.2846980
C	-2.9804500	-2.3914590	-0.9663960
C	-3.7644960	-1.6051150	-0.1887440
H	-3.2166140	-3.2605440	-1.5597660
H	-4.8199240	-1.6566140	0.0267800
C	2.9111430	-2.5941000	-0.2864960
C	3.7436750	-1.5443000	-0.0871420
H	3.1197940	-3.6327330	-0.4874880
H	4.8205200	-1.4924780	-0.0856830
C	1.6166070	-0.7524090	0.0680550
C	-1.6484900	-0.7721620	-0.0649870
N	1.6222460	-2.0987710	-0.1913090
N	2.9503850	-0.4329690	0.1247870
N	-1.6996720	-1.8676840	-0.8774040
N	-2.9426960	-0.6302700	0.3542430
C	-3.4494880	0.3907970	1.2748290
H	-3.5405350	1.3570060	0.7745340
H	-4.4342710	0.0799900	1.6248650
H	-2.7855370	0.4811330	2.1337270
C	3.5488270	0.8854440	0.3662670
H	3.2653620	1.2592750	1.3497630
H	4.6323490	0.7705270	0.3273130
H	3.2350500	1.5939630	-0.3992300
C	0.4580610	-2.9726990	-0.3500290
H	0.8542540	-3.9583330	-0.6003670
H	-0.0678090	-3.0603110	0.6042820
C	-0.5220860	-2.5176380	-1.4447800
H	-0.8771490	-3.3853710	-2.0039900
H	-0.0250900	-1.8498640	-2.1530210
Si	0.3653690	0.6148820	2.5787230
H	1.1916220	2.8345680	-3.6240900
H	0.0379190	1.9464640	3.1541270
H	1.7583700	0.2686270	2.9706870
H	-0.5415550	-0.3967760	3.1964980
C	1.0832400	2.7466680	-2.5385270
C	-0.3956530	2.8432950	-2.1310350
H	1.5233550	1.7913210	-2.2367260
H	1.6774490	3.5459380	-2.0837830
H	-0.9798890	2.0317820	-2.5832770
H	-0.8332450	3.7684770	-2.5340310
Si	-0.8114810	2.9481920	-0.2816010
H	-1.2009350	1.6532170	0.6341490
H	-2.2340400	3.3875620	-0.1866770
H	0.0042530	3.9161420	0.4809160
H	1.1703540	1.6357870	0.5110540

SBM6 - CH1

51

C	1.8567320	-3.4024160	1.8242600
C	0.9893140	-3.1342980	2.8029830

H	2.7141310	-2.7633090	1.6342050
H	1.7637330	-4.2875540	1.2000360
H	0.1469730	-3.7860930	3.0197050
H	1.1071270	-2.2672790	3.4464000
Rh	0.0761230	-0.1671800	0.4364440
C	-0.2027150	3.8790610	-0.4941610
C	0.6753940	3.9763950	0.5305090
H	-0.6295170	4.6350680	-1.1336400
H	1.1632830	4.8365170	0.9599120
C	-3.8350510	-0.7575430	-1.5298340
C	-3.4993810	-2.0468130	-1.2808400
H	-4.7187300	-0.3308160	-1.9776130
H	-4.0302060	-2.9652360	-1.4763100
C	-1.7808670	-0.7484770	-0.5485620
C	0.1604930	1.7827800	0.2986410
N	-2.7744350	0.0180050	-1.0776350
N	-2.2469160	-2.0217630	-0.6835780
N	-0.5151080	2.5324440	-0.6276270
N	0.8909290	2.6930740	1.0105990
C	1.8474360	2.4221430	2.0893050
H	2.7494420	1.9571750	1.6882150
H	2.1046270	3.3747760	2.5535590
H	1.4024130	1.7663270	2.8342860
C	-1.5168910	-3.2293680	-0.3049340
H	-2.1899980	-3.9181830	0.2101810
H	-1.1045040	-3.7218580	-1.1901260
H	-0.7040410	-2.9715880	0.3754730
C	-2.7516880	1.4781230	-1.1398160
H	-3.5571760	1.7758840	-1.8145900
H	-2.9712250	1.8968900	-0.1528420
C	-1.4184160	2.0361880	-1.6679690
H	-1.6197810	2.8885540	-2.3192800
H	-0.9044310	1.2788210	-2.2640020
S	-1.1575220	0.1226420	2.3948790
H	5.9764090	-0.1998360	-2.0200430
H	-1.6295930	-1.2365990	2.7935510
H	-2.3681390	0.9757920	2.2016790
H	-0.4217730	0.7049700	3.5527170
C	5.0829070	-0.8095220	-2.1855330
C	3.8461360	-0.1550470	-1.5389910
H	4.9604250	-0.9236520	-3.2674180
H	5.2811370	-1.8012800	-1.7662590
H	3.6895970	0.8497770	-1.9517070
H	4.0003260	-0.0255520	-0.4607260
Si	2.2642340	-1.1483050	-1.7874340
H	1.3911660	0.0455050	1.2763460
H	2.2949950	-2.4723540	-1.1201190
H	1.9258930	-1.3336950	-3.2231400
H	1.0562380	-0.3983170	-1.2353340

GT1-5a_DCM

39

Rh	0.5299920	-0.8220790	-0.4172730
C	1.4995250	3.2059160	-1.1279840
C	2.5972600	2.6285590	-1.7053290
H	1.2072750	4.2489680	-1.0366660
H	3.4490380	3.0719890	-2.2144510

C	0.4095160	0.8554860	3.5120680
C	0.9900340	-0.3560160	3.7469630
H	0.1380870	1.6593590	4.1915520
H	1.3261330	-0.8177590	4.6716750
C	0.6086080	-0.2070300	1.4966420
C	1.2951690	0.9450570	-0.8993680
N	0.1868230	0.9419940	2.1359240
N	1.1167220	-0.9857900	2.5141210
N	0.7177340	2.1612280	-0.6379320
N	2.4640260	1.2486580	-1.5479490
C	3.4299630	0.2638080	-2.0413900
H	4.4517520	0.6242260	-1.8495010
H	3.2610140	-0.6766560	-1.4975000
H	3.2964540	0.0967730	-3.1228760
C	1.7212160	-2.3102280	2.3455940
H	2.3733520	-2.5121180	3.2076430
H	0.9454020	-3.0913480	2.2864160
H	2.3180060	-2.3156520	1.4224700
C	-0.4163680	2.1793380	1.5930550
H	-1.4276690	2.2811660	2.0253530
H	0.1961940	3.0199640	1.9643250
C	-0.5558730	2.2736670	0.0739670
H	-0.9987750	3.2554720	-0.1587330
H	-1.2330170	1.4966650	-0.3115580
Si	0.4899140	-2.8476170	-1.4975900
H	0.5826950	-1.3641640	-2.1512130
H	1.7394860	-3.6601780	-1.5993020
H	-0.6219420	-3.5402190	-2.2098290
H	0.0024310	-2.5766140	0.0047720
C	-4.0987370	-0.5893010	-0.9176640
H	-4.3081190	-0.5639670	-1.9936970
H	-4.5308740	-1.4676970	-0.4237510
Cl	-2.2506640	-0.7217070	-0.7301290
Cl	-4.7584180	0.8860490	-0.1622270

GT4-5a_DCM

50

Rh	-0.2666430	0.4179190	-0.0839310
C	-4.1563050	0.4448630	-1.5793800
C	-4.0864050	1.7480630	-1.1728500
H	-4.9589530	-0.1103230	-2.0581900
H	-4.8195370	2.5489210	-1.2236900
C	-2.2433510	-2.8547080	2.0491820
C	-1.4619790	-2.3417520	3.0428380
H	-2.9413420	-3.6882420	2.0490040
H	-1.3489870	-2.6358360	4.0831190
C	-1.0628310	-1.0990290	1.1537370
C	-2.0773600	0.7871470	-0.6936130
N	-1.9985880	-2.0888000	0.9104740
N	-0.7594810	-1.2796580	2.4886610
N	-2.9199320	-0.1277680	-1.2813910
N	-2.8140680	1.9441080	-0.6334100
C	-2.3460910	3.2207010	-0.0866250
H	-3.0274160	3.5595170	0.7095660
H	-1.3420100	3.0625720	0.3309840
H	-2.3012760	3.9812520	-0.8824960
C	0.1750960	-0.4653770	3.2753690
H	0.1304350	-0.8014980	4.3207280

H	1.2026400	-0.5866580	2.9032820
H	-0.1142340	0.5945040	3.2309890
C	-2.7319730	-2.4289120	-0.3281520
H	-2.4390300	-3.4513880	-0.6283110
H	-3.8050540	-2.4537170	-0.0683970
C	-2.5141200	-1.5102490	-1.5275750
H	-3.1080190	-1.9046670	-2.3684570
H	-1.4542220	-1.4960500	-1.8246970
Si	1.8373650	2.4746300	1.7437520
H	0.6459460	3.3133610	2.1023960
H	4.8909890	2.3507690	1.1775520
H	2.5028890	2.0216630	3.0103680
H	1.2453940	1.1938150	1.1200980
C	3.0272320	3.3538400	0.5658500
C	4.3227360	2.5725600	0.2584490
H	3.2660140	4.3301670	1.0297210
H	2.4805100	3.5876360	-0.3665110
H	4.1111610	1.6145000	-0.2451780
H	4.9826370	3.1568810	-0.4044350
Si	0.4584860	0.6433030	-2.3243030
H	0.2639960	1.7564040	-0.8592960
H	1.8522080	1.1465410	-2.5533520
H	-0.4600390	1.3912360	-3.2429150
H	0.4577640	-0.7922570	-2.8179410
Cl	2.3889760	-1.1064860	0.1451130
C	2.6616150	-2.4766500	-1.0351800
H	2.4787370	-3.4075140	-0.4847490
H	1.9482330	-2.3223910	-1.8551250
Cl	4.3124650	-2.4967370	-1.6864120

GT5a_DCM

39

Rh	-0.1899320	-0.4095030	-0.2734300
C	3.8535980	-1.1493080	-0.7825520
C	3.7199240	-1.9541410	0.3132130
H	4.7184970	-0.9238810	-1.4013460
H	4.4461690	-2.5704600	0.8367570
C	1.9061780	3.3169050	0.4437340
C	1.0399620	3.3320600	1.4999380
H	2.6701890	4.0277680	0.1385720
H	0.9084360	4.0538100	2.3021820
C	0.6307040	1.4246800	0.3143340
C	1.6601130	-1.0840760	-0.1273750
N	1.6486020	2.1448570	-0.2707370
N	0.2743650	2.1738950	1.4059510
N	2.5877840	-0.6256530	-1.0378570
N	2.3806040	-1.8955090	0.7104030
C	1.8738540	-2.5877660	1.8995020
H	2.6236990	-2.5147970	2.7017380
H	0.9491090	-2.0950680	2.2272500
H	1.6711150	-3.6474790	1.6805230
C	-0.7592160	1.7954890	2.3769850
H	-0.3383150	1.8148900	3.3943410
H	-1.6125410	2.4893610	2.3179000
H	-1.0933520	0.7758850	2.1368880
C	2.4037770	1.8271680	-1.5011470
H	2.0926860	2.5239660	-2.3005270

H	3.4678160	2.0224420	-1.2825000
C	2.2390400	0.3946010	-2.0271880
H	2.8845400	0.2771750	-2.9132990
H	1.1940950	0.1973000	-2.3311390
Si	-1.2866570	-2.3711860	0.5054360
H	-0.6427950	-1.7607550	-1.0727730
H	-0.5843790	-3.6918650	0.4198600
H	-2.6765290	-2.5868030	-0.0228650
H	-1.4324940	-2.0367530	1.9711540
C	-3.8004830	-0.0745030	-1.2520430
H	-4.2599710	0.4892280	-2.0731540
H	-3.4775440	-1.0807060	-1.5459110
Cl	-2.2515070	0.8636050	-0.8549140
Cl	-4.9127560	-0.1676530	0.1164360

GT5a_DCM-CH1

45

Rh	0.1000450	0.0516820	0.5642050
C	-2.4463840	-2.5688710	-1.6526120
C	-1.3518180	-2.7091670	-2.4618030
H	-3.4381370	-3.0106250	-1.7115660
H	-1.2048740	-3.2970310	-3.3643830
C	-3.1036020	2.4377690	-0.7634950
C	-2.0525510	3.2888920	-0.9374150
H	-4.1645260	2.5660770	-0.9621700
H	-2.0140000	4.3026110	-1.3274330
C	-1.2159620	1.3441980	-0.0741970
C	-0.7552930	-1.3053590	-0.7633480
N	-2.5883530	1.2506970	-0.2364220
N	-0.9111350	2.6133880	-0.5189520
N	-2.0624540	-1.7075160	-0.6279080
N	-0.3361020	-1.9271040	-1.9107090
C	0.9997590	-1.8074880	-2.5038160
H	0.9075660	-1.5589220	-3.5723520
H	1.5434950	-1.0037970	-1.9915200
H	1.5554170	-2.7526100	-2.3948200
C	0.4321180	3.2009800	-0.5409020
H	0.4193680	4.0751340	-1.2080120
H	0.7273230	3.5199610	0.4717150
H	1.1530250	2.4616780	-0.9175760
C	-3.5239510	0.1696060	0.1399140
H	-4.0911130	0.4928920	1.0318840
H	-4.2388030	0.0717560	-0.6954250
C	-2.9053500	-1.1957590	0.4517620
H	-3.7287970	-1.9069710	0.6298890
H	-2.2836360	-1.1409210	1.3576900
Si	-0.3791930	0.9080460	2.7219170
H	0.5881620	0.4850140	3.7882340
H	-1.7106040	0.2737790	3.0639170
H	-0.6075470	2.3844790	2.8694950
C	3.9913510	0.6591990	-0.0228780
H	0.8896840	1.1958920	1.4370280
H	5.0384100	0.3390750	0.0418540
Cl	3.6661370	1.2043040	-1.6962120
Cl	2.9808880	-0.7601310	0.4820850
H	3.7639500	1.4818600	0.6657980
C	1.3959140	-2.6677540	2.3995370
C	0.0520060	-2.6010570	2.3108940

H	-0.5422540	-2.0596240	3.0540650
H	-0.4990750	-3.1639750	1.5506410
H	1.9871530	-3.2745420	1.7049150
H	1.9459250	-2.1478610	3.1903150