Electronic Supplementary Material (ESI) for Chemical Science.

Supporting Information

Carbon Dioxide Reduction by an Al–O–P Frustrated Lewis Pair

Lucas Wickemeyer[a], Niklas Aders[a], Andreas Mix[a], Beate Neumann[a], Hans-Georg Stammler[a], Jorge Juan Cabrera-Trujillo[b], Israel Fernandéz-Lopéz[b] and Norbert W. Mitzel*[a]

[a] Lehrstuhl für Anorganische Chemie und Strukturchemie and Centrum für Molekulare Materialen CM_2
Fakultät für Chemie, Universität Bielefeld
Universitätsstraße 25, 33615 Bielefeld (Germany)
E-mail: mitzel@uni-bielefeld.de

[b] Departamento de Química Orgánica I
Facultad de Ciencias Químicas, Universidad Complutense de Madrid
28040 Madrid (Spain)

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1) NMR spectra

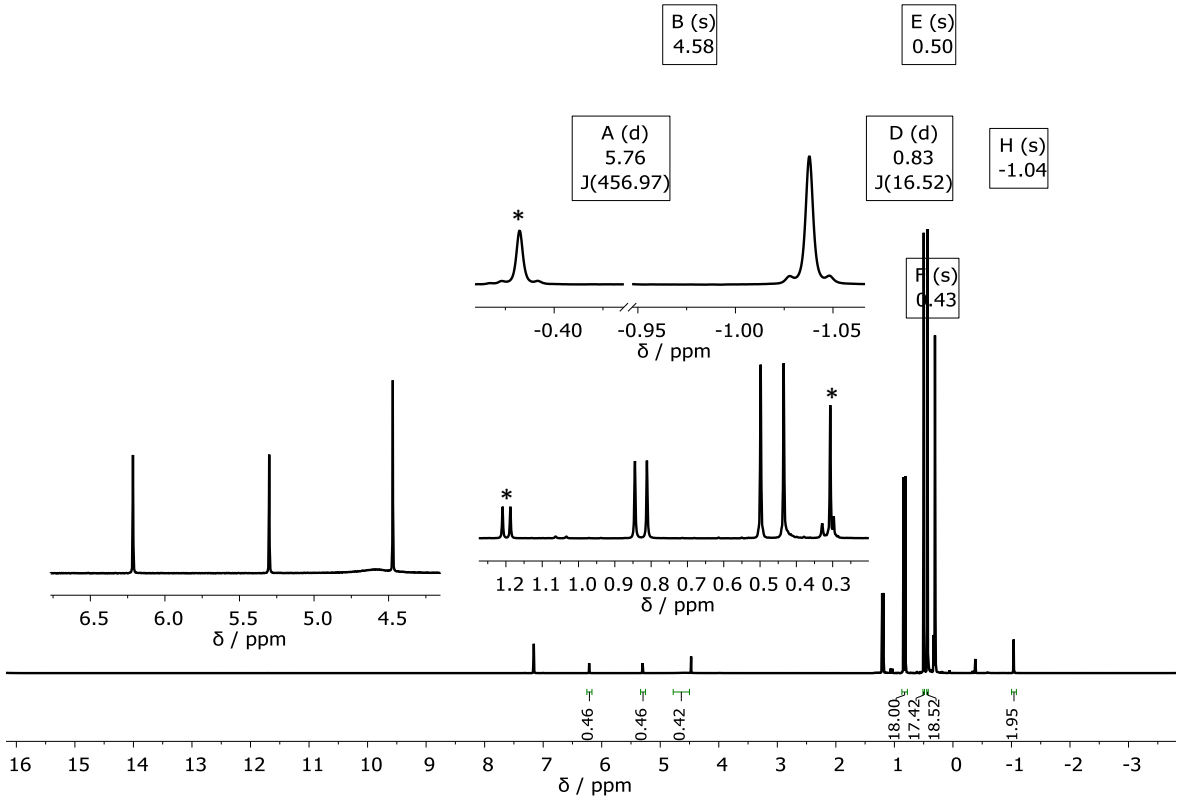

Figure S1. ^{1}H NMR of ^{t}Bu$_2$P(H)(O)Al(H)Bis$_2$ (**3**), 15 min after mixing *t*Bu$_2$P(O)H and Bis$_2$AlH in C_6D_6 (500 MHz, 293 K). About 27 % of FLP **4** are formed, the signals are denoted with *.

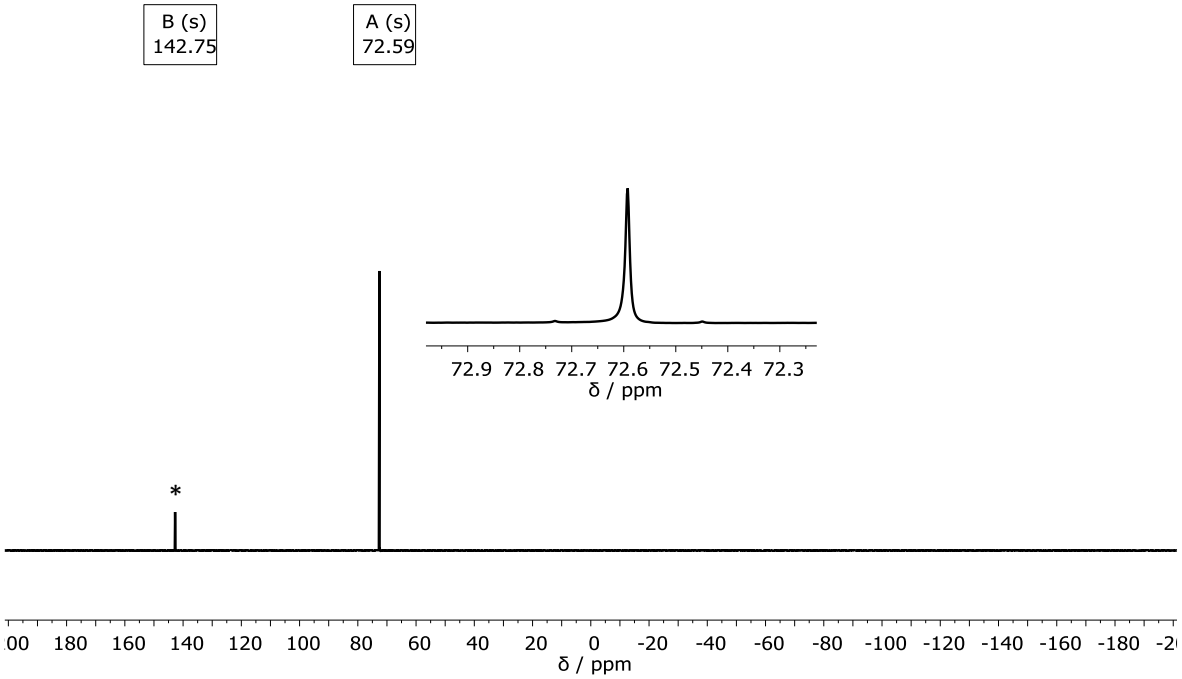

Figure S2. ^{31}P{^{1}H} NMR spectrum of ^{t}Bu$_2$P(H)(O)Al(H)Bis$_2$ (**3**), 15 min after mixing *t*Bu$_2$P(O)H and Bis$_2$AlH in C_6D_6 (202 MHz, 293 K). About 27 % of FLP **4** are formed, the signals are denoted with *.

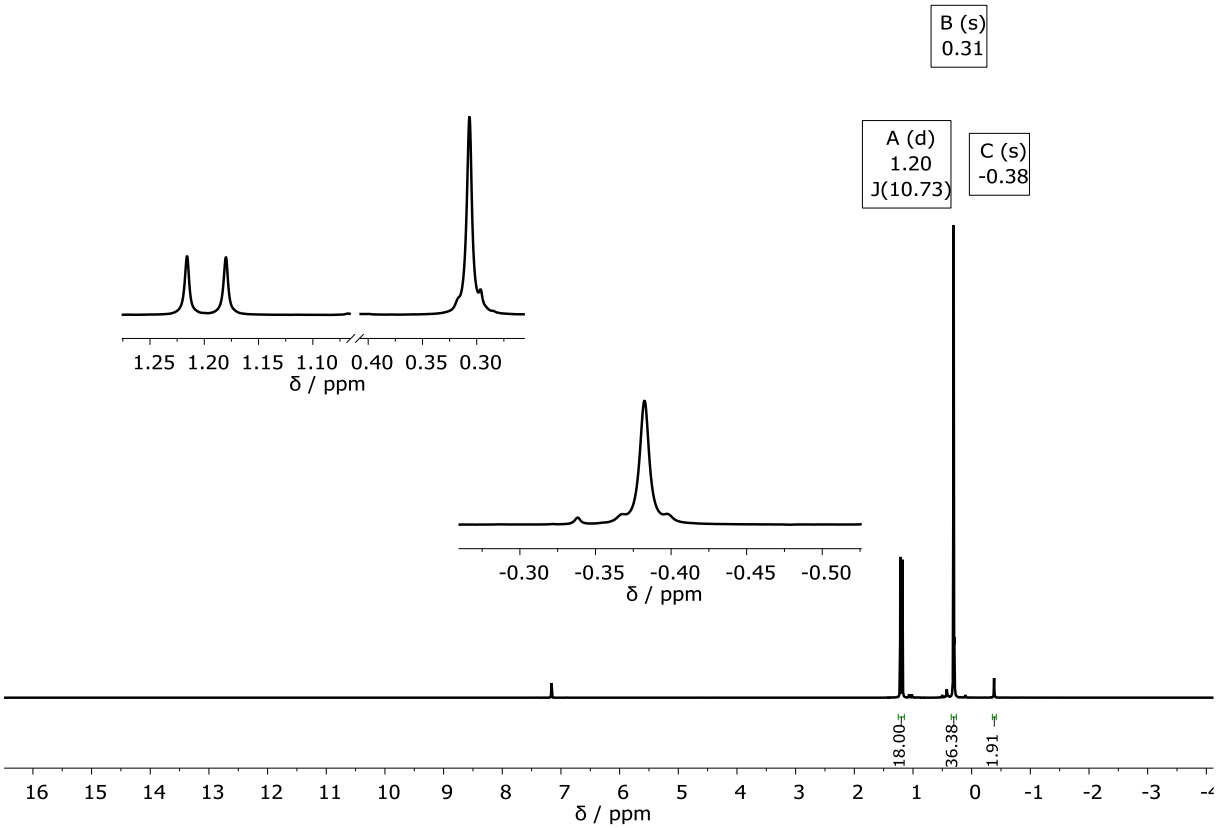

Figure S3. ^{1}H NMR spectrum of $^{t}Bu_2P(O)AlBis_2$ (**4**) in C_6D_6 (300 MHz, 293 K).

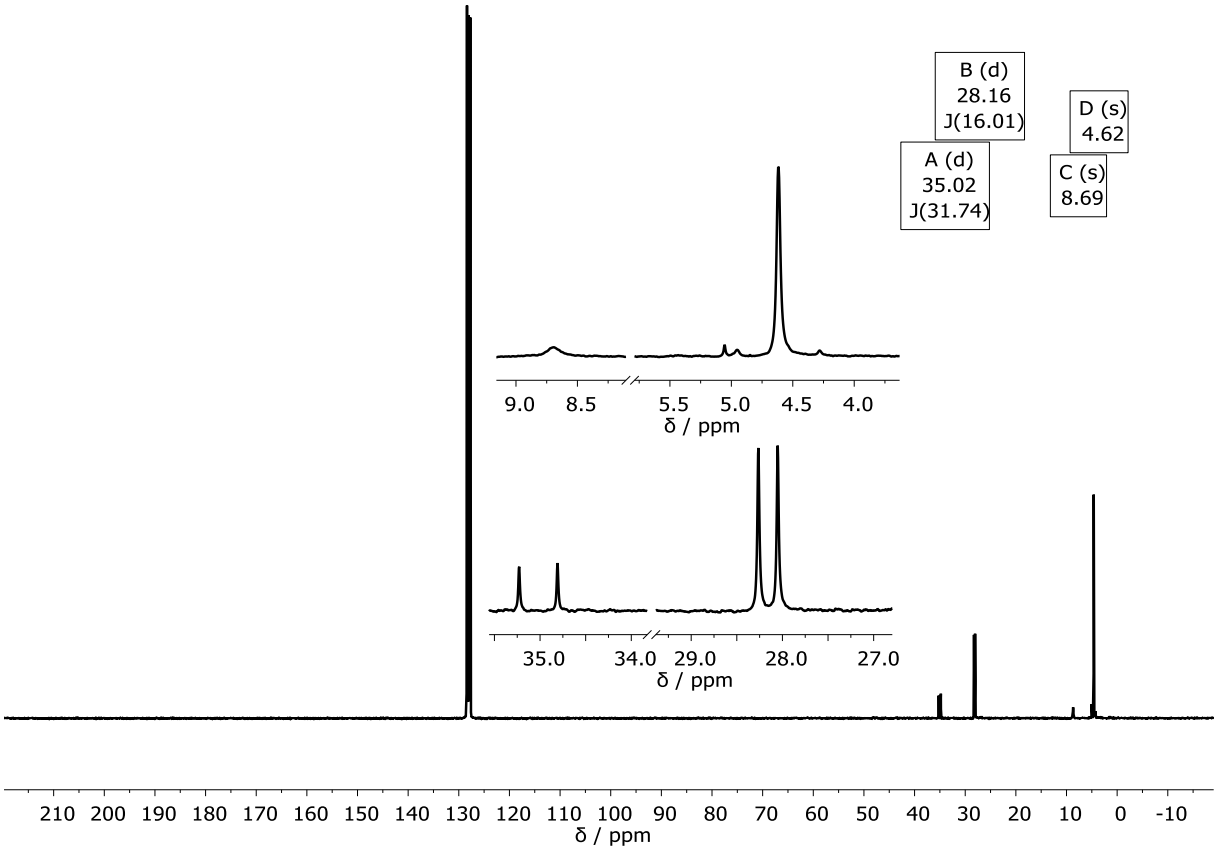

Figure S4. $^{13}C\{^{1}H\}$ NMR spectrum of $^{t}Bu_2P(O)AlBis_2$ (**4**) in C_6D_6 (75 MHz, 293 K).

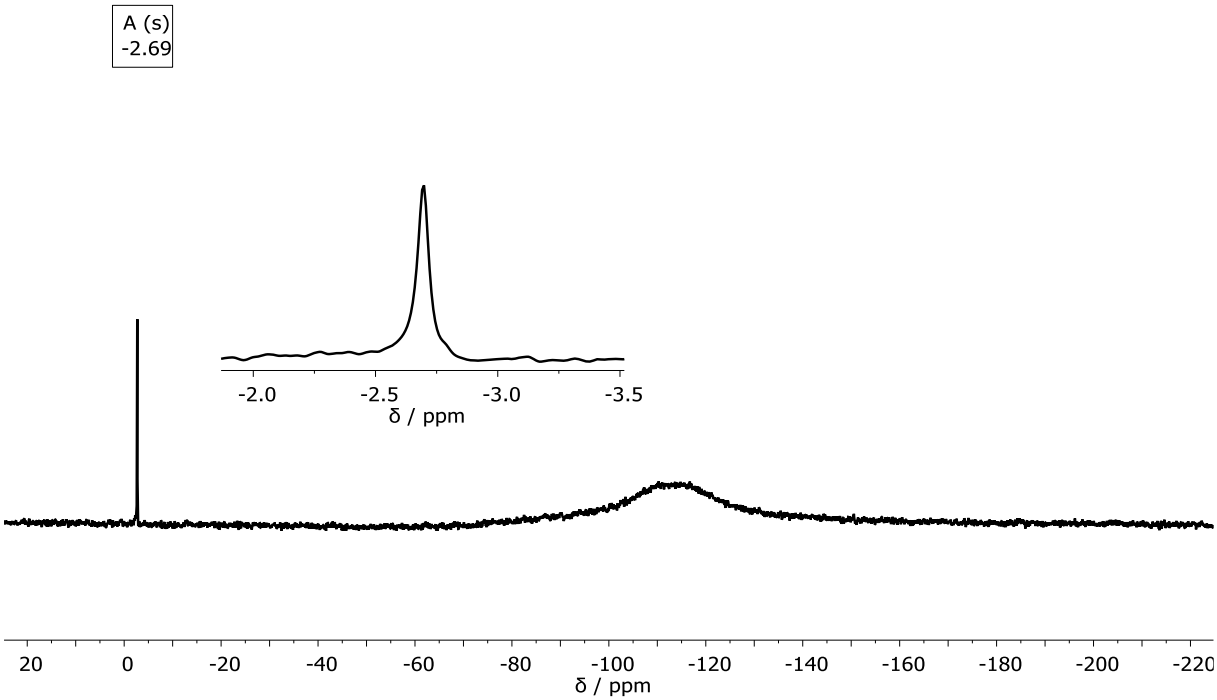

Figure S5. $^{29}Si\{^{1}H\}$ NMR spectrum of $^{t}Bu_2P(O)AlBis_2$ (**4**) in C_6D_6 (60 MHz, 293 K).

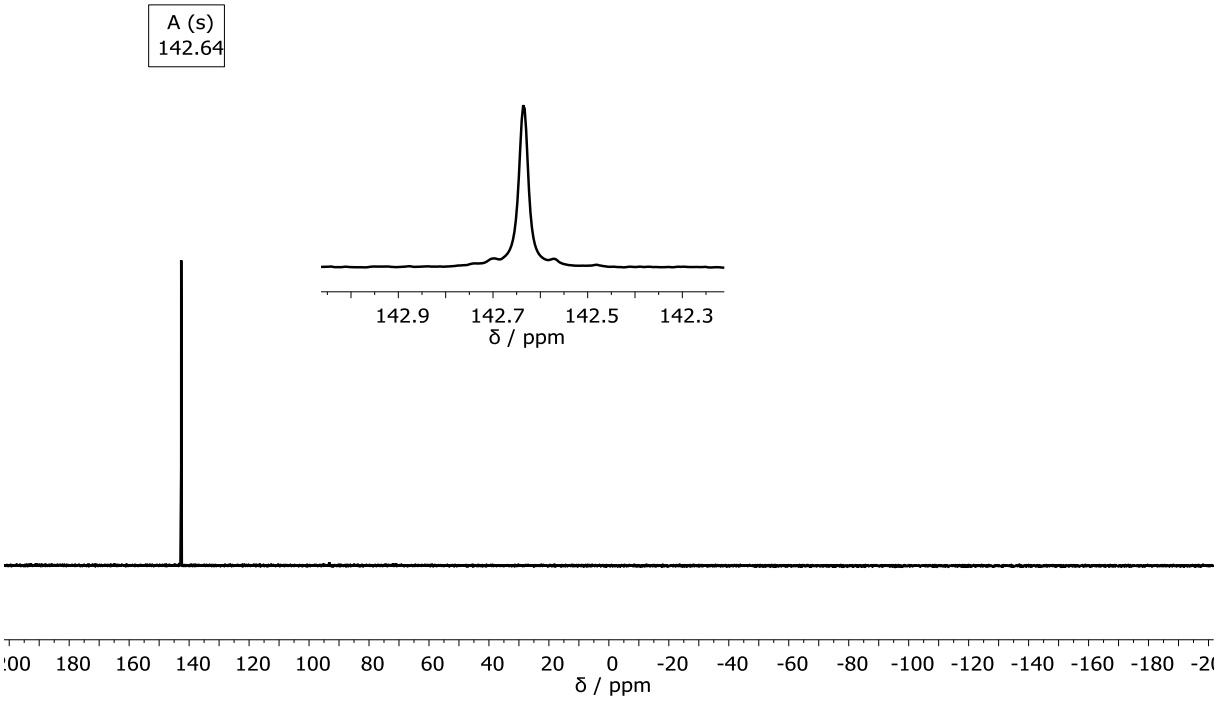

Figure S6. $^{31}P\{^{1}H\}$ NMR spectrum of $^{t}Bu_2P(O)AlBis_2$ (**4**) in C_6D_6 (121 MHz, 293 K).

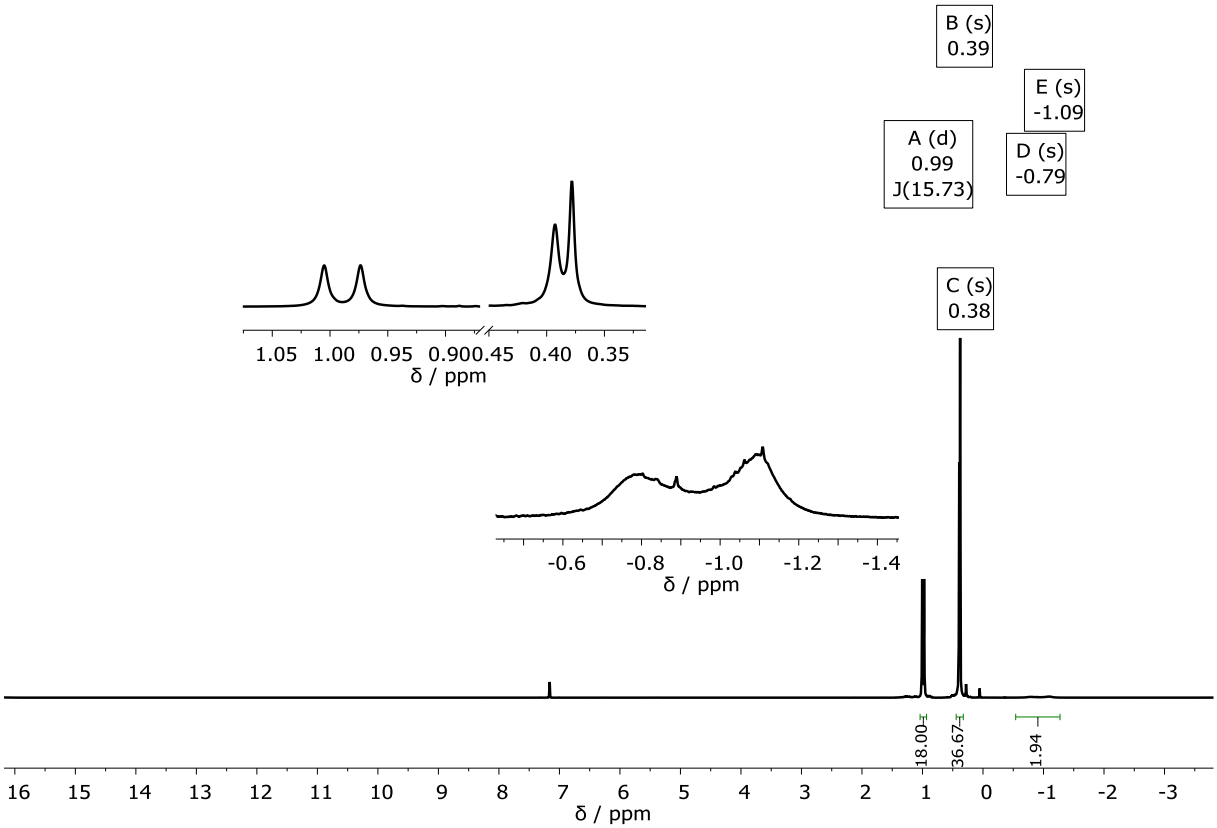

Figure S7. ^{1}H NMR spectrum of $^{t}Bu_2P(O)AlBis_2{\cdot}CO_2$ (**5**) in C_6D_6 (500 MHz, 293 K).

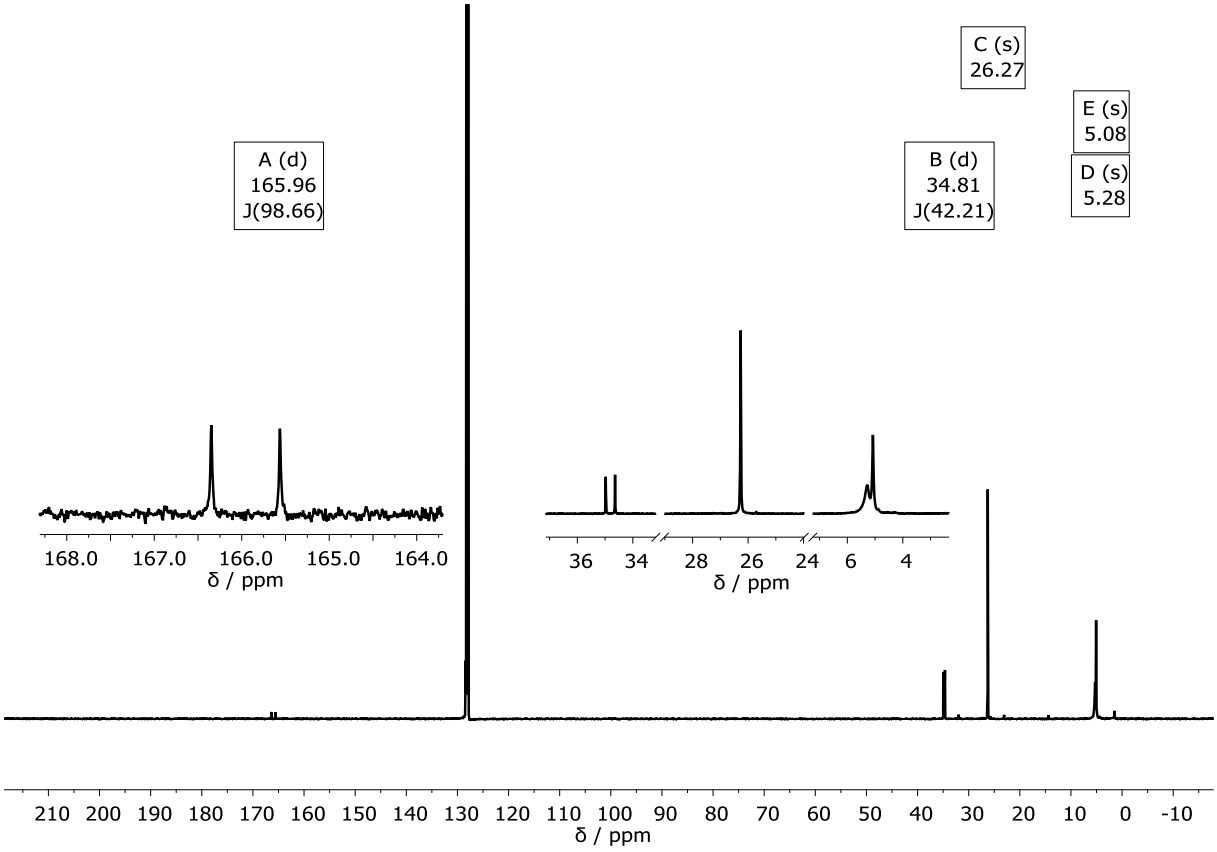

Figure S8. $^{13}C\{^{1}H\}$ NMR spectrum of $^{t}Bu_2P(O)AlBis_2{\cdot}CO_2$ (**5**) in C_6D_6 (126 MHz, 293 K).

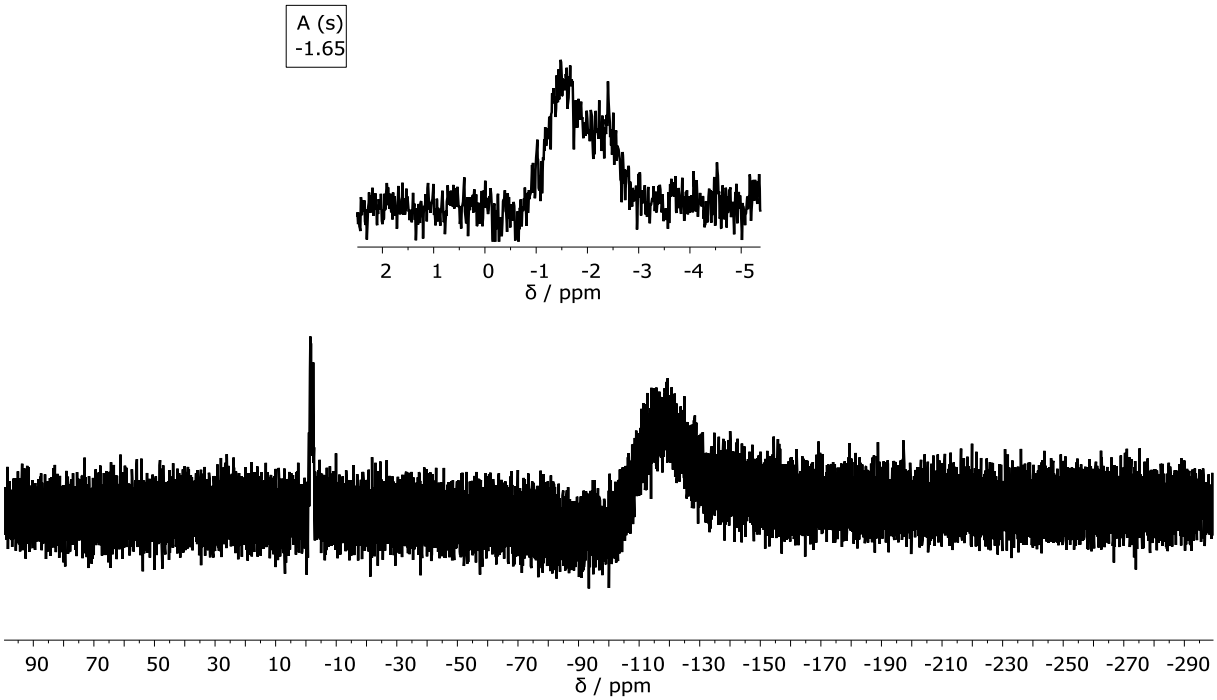

Figure S9. $^{29}Si\{^{1}H\}$ NMR spectrum of $^{t}Bu_2P(O)AlBis_2{\cdot}CO_2$ (**5**) in C_6D_6 (99 MHz, 293 K).

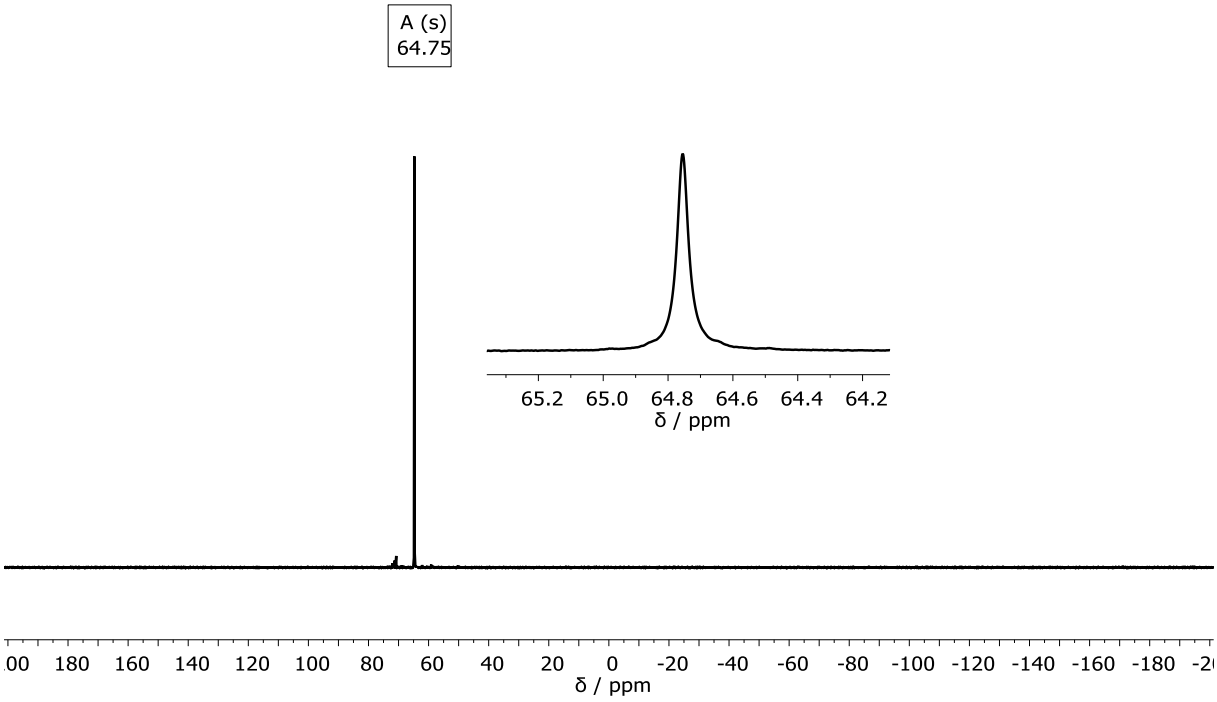

Figure S10. $^{31}P\{^{1}H\}$ NMR spectrum of $^{t}Bu_2P(O)AlBis_2{\cdot}CO_2$ (**5**) in C_6D_6 (202 MHz, 293 K).

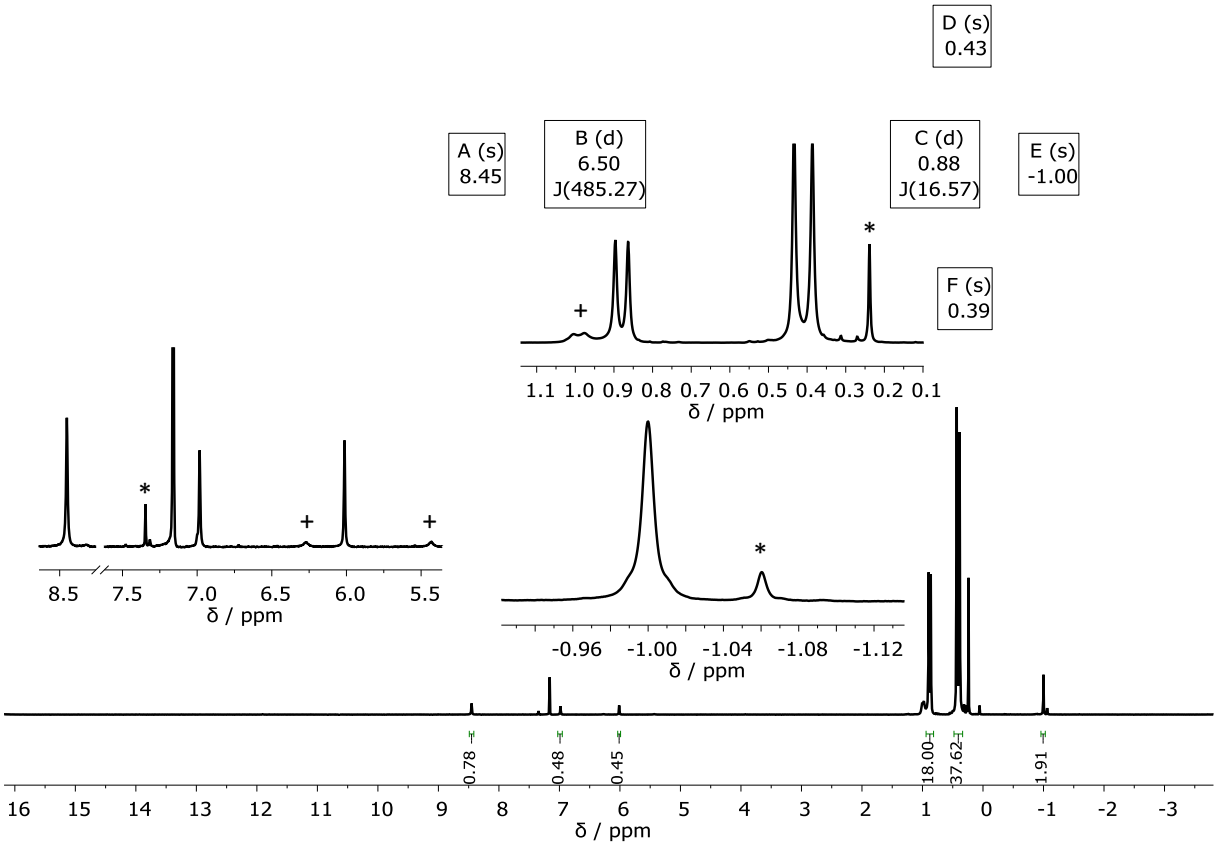

Figure S11. ^{1}H NMR spectrum of *t*Bu$_2$P(H)(O)Al(CO$_2$H)Bis$_2$ (**6**) in C$_6$D$_6$ (500 MHz, 293 K). * denotes the signals of free BisAlCO$_2$H, + denotes free phosphine oxide.

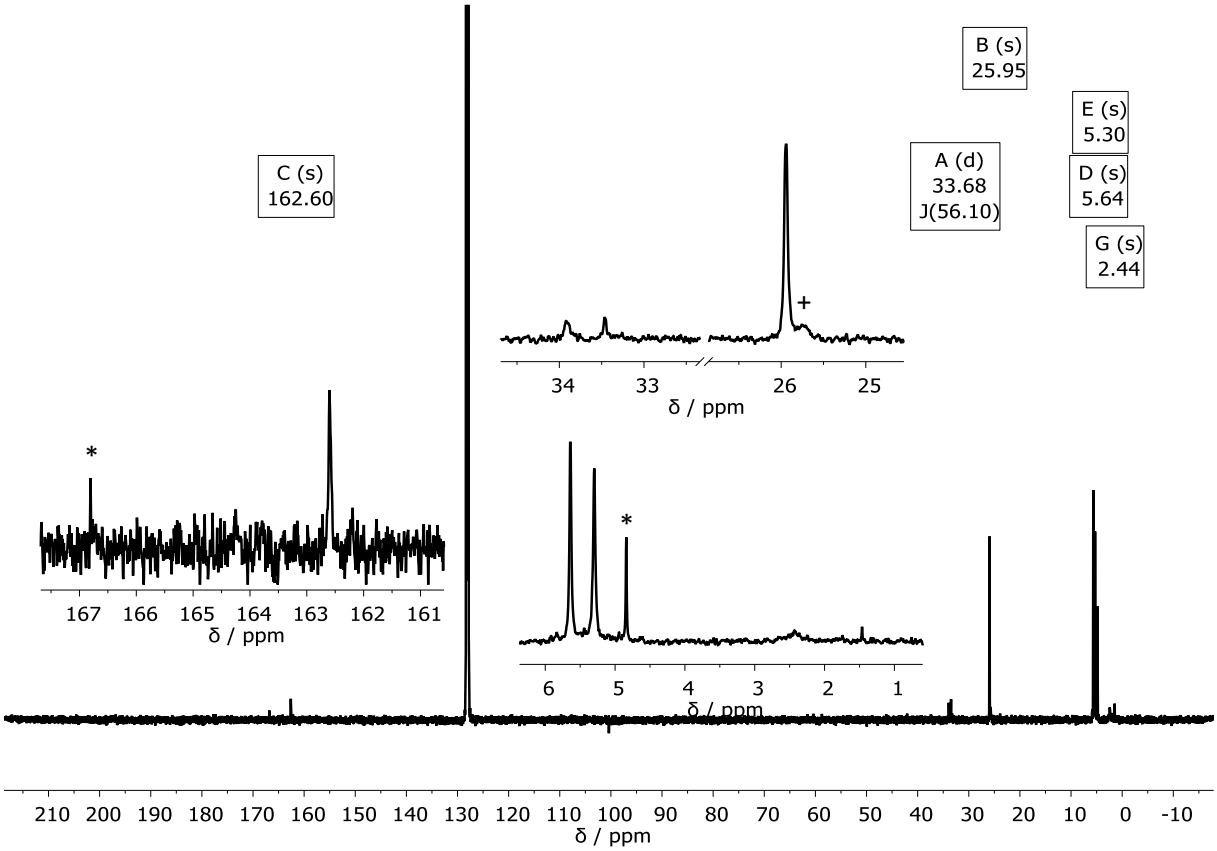

Figure S12. ^{13}C{^{1}H} NMR spectrum of *t*Bu$_2$P(H)(O)Al(CO$_2$H)Bis$_2$ (**6**) in C$_6$D$_6$ (126 MHz, 293 K). * denotes the signals of free BisAlCO$_2$H, + denotes free phosphine oxide.

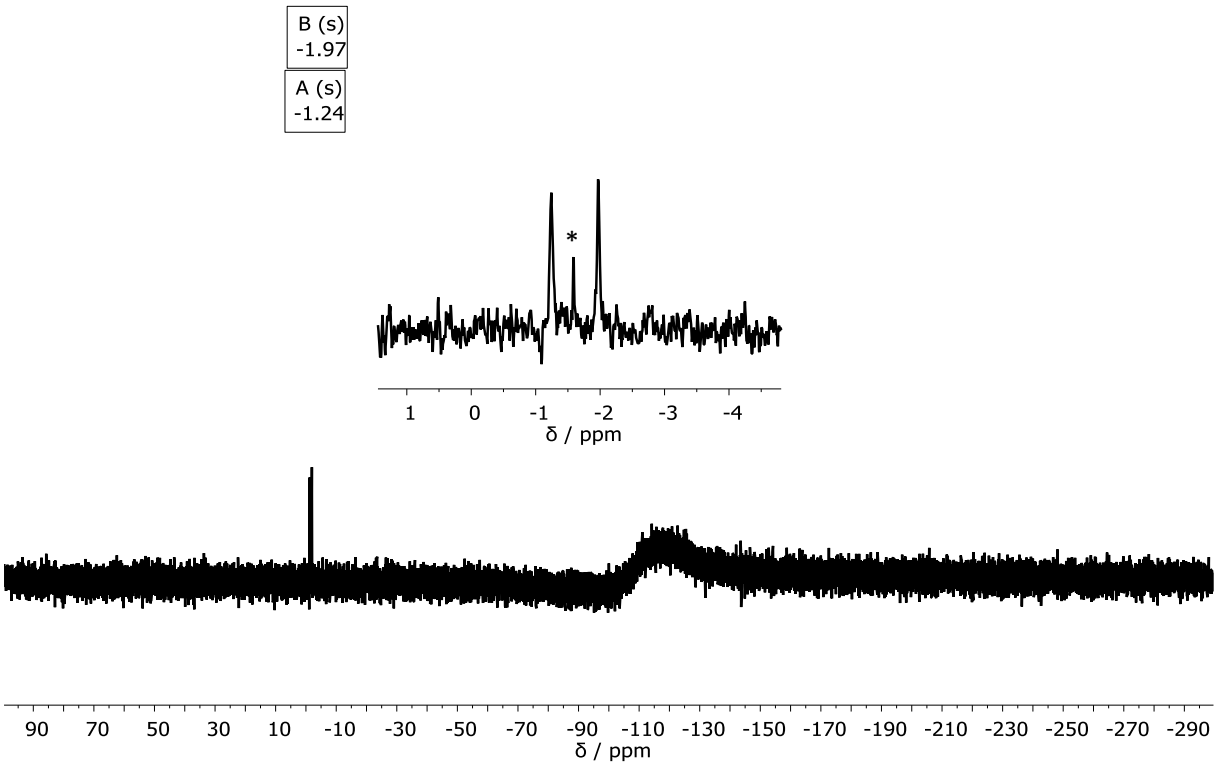

Figure S13. $^{29}Si\{^{1}H\}$ NMR spectrum of *t*$Bu_2P(H)(O)Al(CO_2H)Bis_2$ (**6**) in C_6D_6 (99 MHz, 293 K). * denotes the signals of free $BisAlCO_2H$.

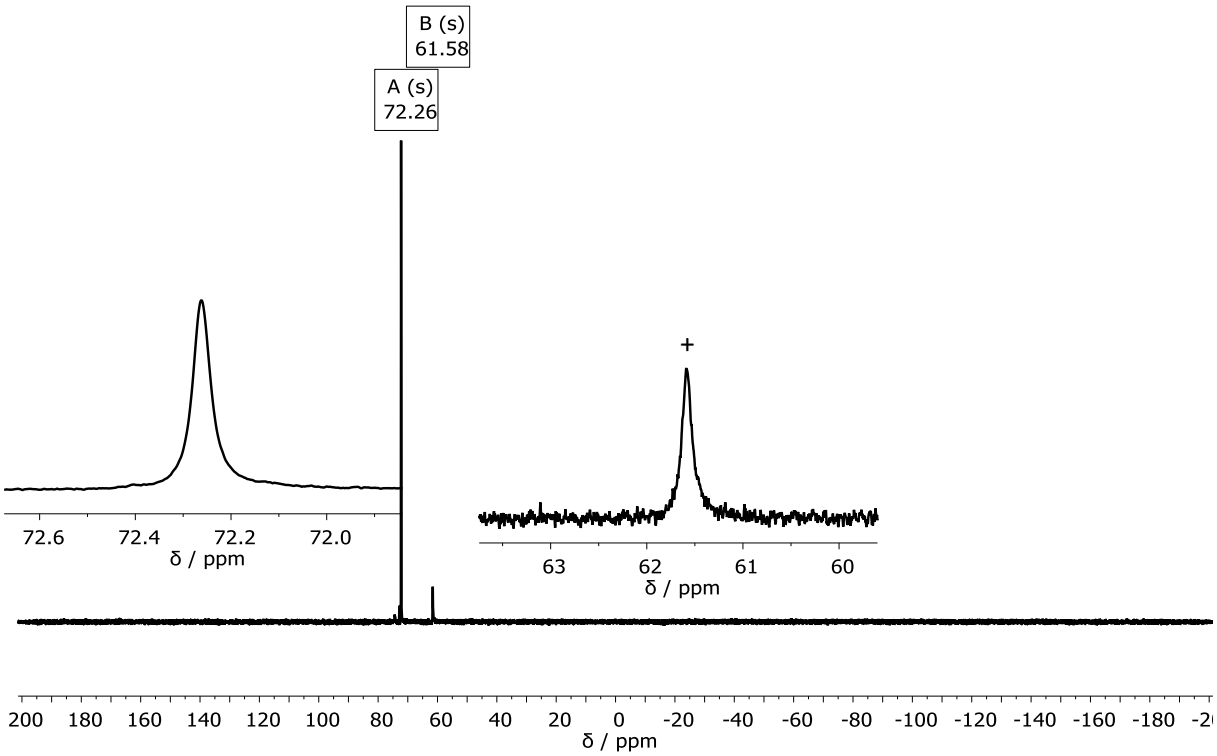

Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum of *t*$Bu_2P(H)(O)Al(CO_2H)Bis_2$ (**6**) in C_6D_6 (202 MHz, 293 K). + denotes the signals of free phosphine oxide.

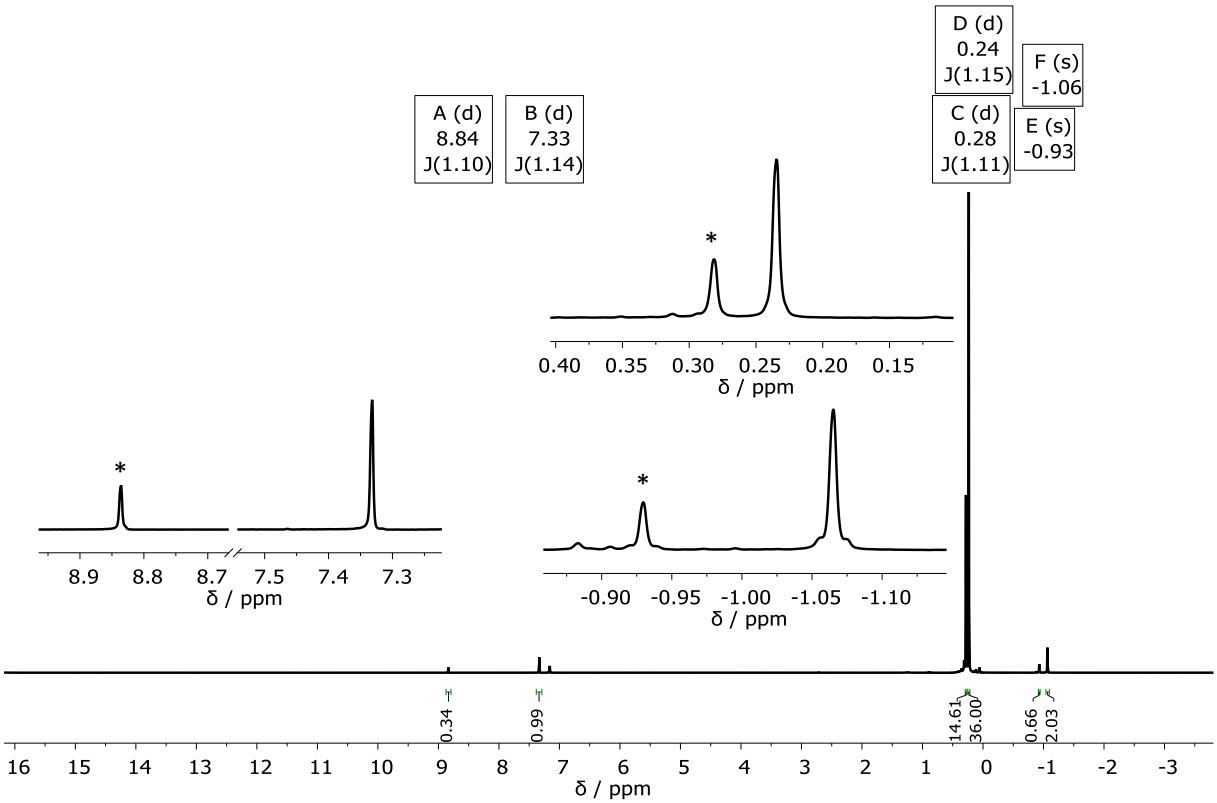

Figure S15. ^{1}H NMR spectrum of $Bis_2Al(CO_2H)$ (**7**) and $(Bis_2Al(CO_2H))_2$ (**7d**) in C_6D_6 (500 MHz, 293 K). * denotes the signals of the dimeric species **7d**.

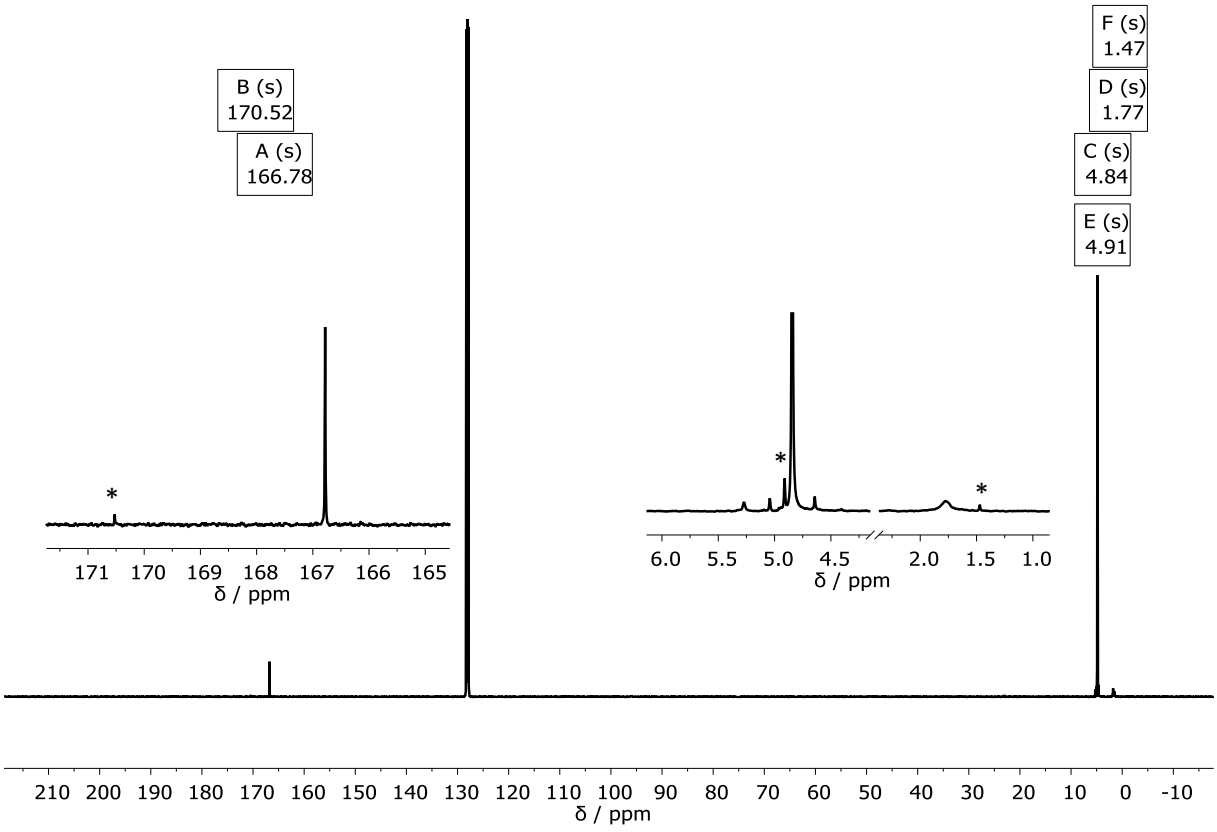

Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of $Bis_2Al(CO_2H)$ (**7**) and $(Bis_2Al(CO_2H))_2$ (**7d**) in C_6D_6 (126 MHz, 293 K). * denotes the signals of the dimeric species **7d**.

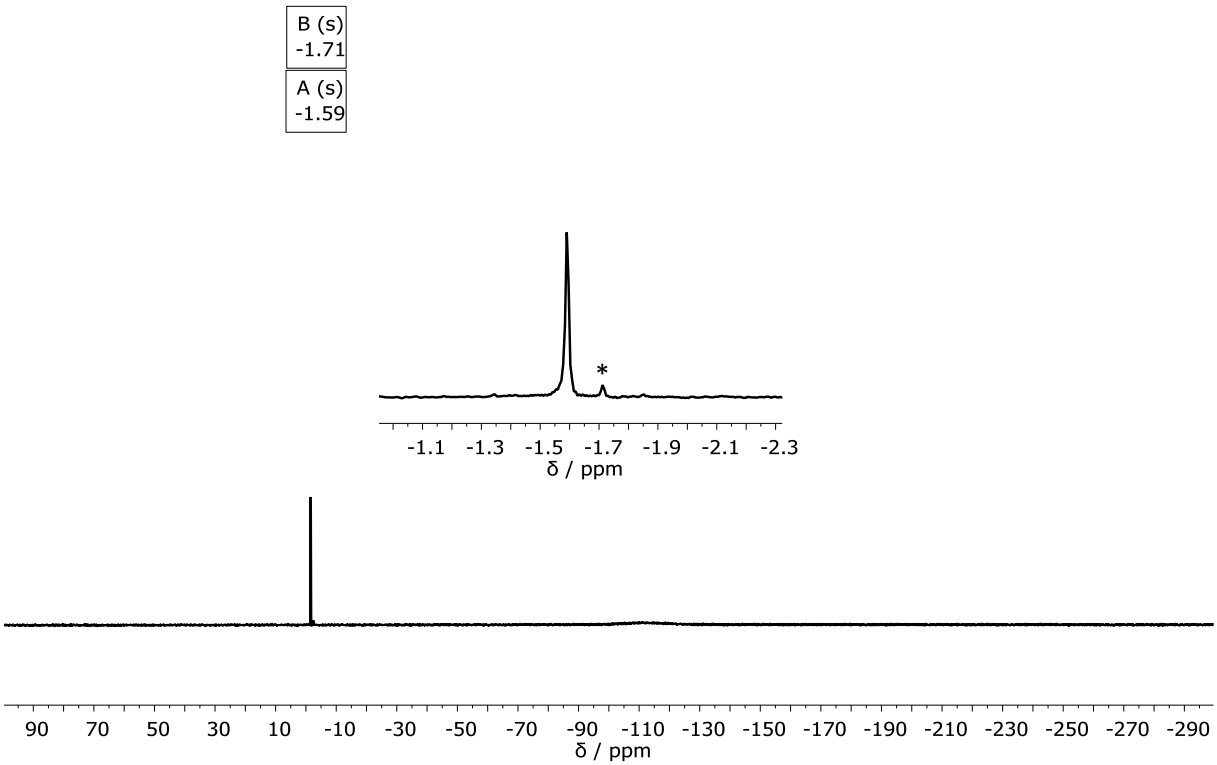

Figure S17. $^{29}Si\{^{1}H\}$ NMR spectrum of $Bis_2Al(CO_2H)$ (**7**) and $(Bis_2Al(CO_2H))_2$ (**7d**) in C_6D_6 (99 MHz, 293 K). * denotes the signals of the dimeric species **7d**.

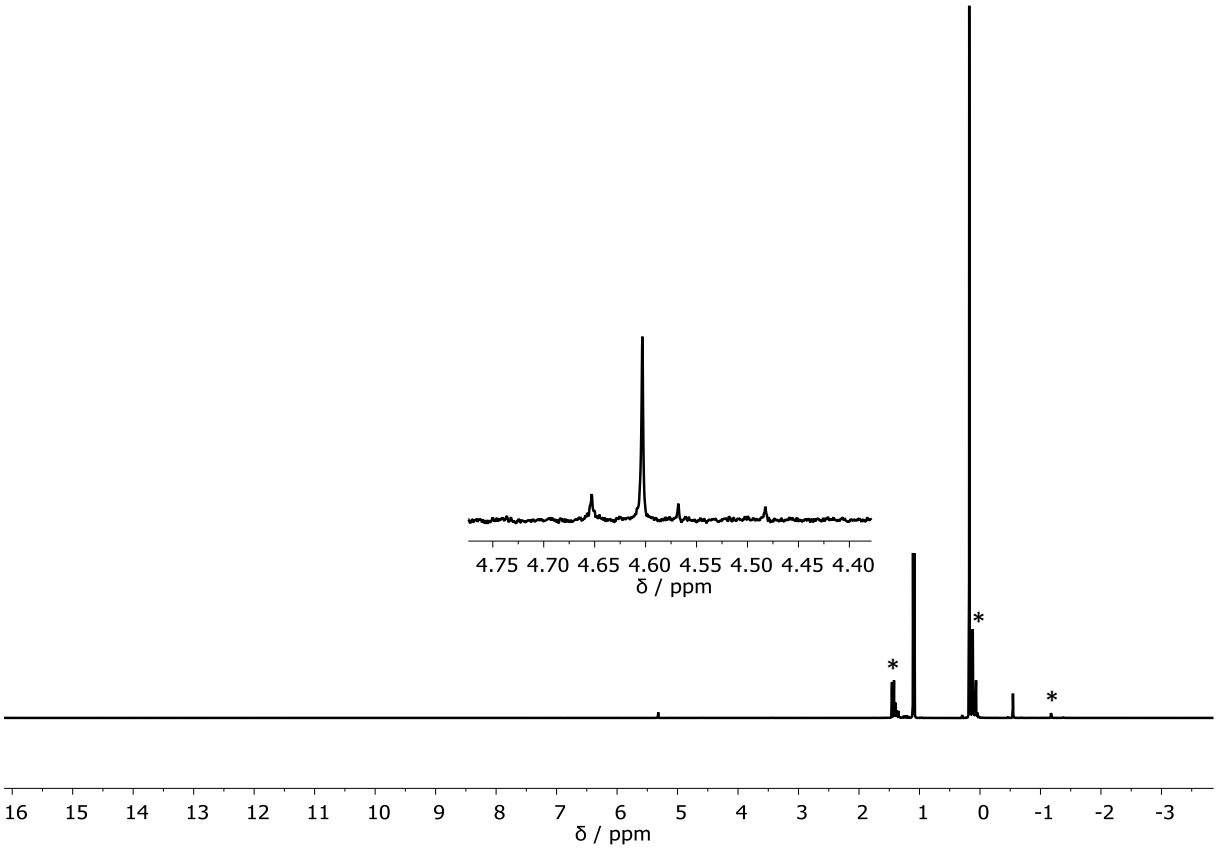

Figure S18. ^{1}H NMR spectrum of $^{t}Bu_2P(O)AlBis_2$ (**4**) with a mixture of H_2/D_2 (1:1, 1 bar) after two weeks (CD_2Cl_2, 500 MHz). * denotes the signals of $^{t}Bu_2P(H/D)(O)Al(H/D)Bis_2$ (**3**)

2) Diffusion NMR experiments

Diffusion NMR experiments have been performed on a Bruker Avance *NEO* 600 FT NMR spectrometer, operating at a ^{1}H resonance frequency of 600.13 MHz. The instrument was equipped with a 5 mm BBO Prodigy cryoprobe exhibiting a *z*-gradient coil delivering a maximum gradient strength of 6.57 G mm^{-1} at 10 A. Diffusion data have been recorded using the *dstebpgp3s* pulse sequence delivered by the manufacturer. Diffusion coefficients have been corrected according to the diffusion coefficient of H_2O (2.299×10^{-9} m^2 s^{-1} at 298 K) reported in the literature.[1] The corresponding proportional factor $D_{H2O,lit.}/D_{H2O,est.}$ was determined on a sample of acetone-d_6 equipped with a capillary containing H_2O. The temperature unit of the instrument was calibrated according to the manual of the manufacturer of the instrument using the temperature dependence of the proton chemical shift difference of methanol. In order to obtain stable temperature conditions, the sample was kept within the magnet for at least one hour at the respective temperature prior to data collection. Proton diffusion data have been collected with 32k data points and a spectral width of 7100 Hz. The relaxation delay was set to 10 s. The diffusion delay time (big Delta, Δ) was set to 50 ms. The gradient duration time (little delta, $\delta/2$) has been set to 1400 μs. The gradient strength within the diffusion experiments was incremented linearly using 16 steps. The diffusion data have been analysed with the *T*1/*T*2 module which is part of the Bruker *TopSpin*® software package. The standard deviation of the experimentally determined gradient strength dependent signal intensities to the fitted decay function was ≤ 2.54 x 10^{-3}.

The hydrodynamic radii have been calculated by the Stokes-Einstein equation, (eq. 1 and the hydrodynamic Volume have been calculated by equation for a spherical volume (eq. 2):

$$D = \frac{k_B T}{6\pi\eta r_H} \qquad r_H = \frac{k_B T}{6\pi\eta D} \quad \text{(eq. 1)} \qquad\qquad V_H = \frac{4}{3}\pi r_H^3 \quad \text{(eq. 2)}$$

D = diffusion constant

k_B =Boltzmann constant

T = temperature

η = viscosity

3) Crystallographic data

Single crystals were examined on a Rigaku Supernova diffractometer. The crystals were kept at 100.0(1) K resp. 220.0(1) K during data collection. Using Olex2[2], the structure was solved with the ShelXT[3] structure solution program using Intrinsic Phasing and refined with the ShelXL[4] refinement package using Least Squares minimization. The crystal structure of **4** shows a heavy positional disorder of one O–AlBis group with the O–P*t*Bu$_2$ group with ratio 93:7 and C(2) and C(1b) with a ratio of 65:35. Suitable constraints and restraints were applied. The HC(SiMe$_3$)$_2$ groups in the structure of **5** are heavily disordered with ratio 1:1, suitable restraints were used. The structure of **6** adduct shows a disorder of C(24) with ratio 77:23. The hydrogen atoms bound to P in this structure were refined isotropically, all others were taken into account using a riding model. Details of the X-ray investigation are given in Table S1. CCDC 2151906-2151909 contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/conts/retrieving.html.

Table S1: Crystallographic data for compounds

Compound	**4**	**5**	**6**	**7d**
Empirical formula	$C_{22}H_{56}AlOPSi_4$	$C_{23}H_{55}AlO_3PSi_4$	$C_{23}H_{58}AlO_3PSi_4$	$C_{30}H_{78}Al_2O_4Si_8$
M_r	506.97	549.98	553.00	781.60
T [K]	100.0(1)	220.0(1)	100.0(1)	100.0(1)
Radiation	Cu Kα	Mo Kα	Cu Kα	Cu Kα
Crystal system	triclinic	monoclinic	triclinic	monoclinic
Space group	$P\bar{1}$	$P2_1/n$	$P\bar{1}$	$P2_1/n$
a [Å]	9.05033(13)	11.738(2)	12.51484(16)	14.9120(3)
b [Å]	11.72687(18)	28.6426(13)	16.89311(17)	9.33098(17)
c [Å]	16.30904(19)	11.8207(18)	17.04953(18)	17.8266(5)
α [°]	94.4336(11)	90	84.6973(8)	90
β [°]	96.4467(11)	119.12(2)	76.7333(10)	104.662(3)
γ [°]	108.8844(14)	90	75.2570(10)	90
Volume [Å^3]	1615.45(4)	3471.9(10)	3390.60(7)	2399.69(10)
Z	2	4	4	2
ρ_{calc} [g/cm^3]	1.042	1.052	1.083	1.082
μ [mm^{-1}]	2.513	0.262	2.477	2.681
F(000)	560	1204	1216	856
2Θ range [°]	5.494–153.262	4.864 – 60.052	5.328–152.972	11.746–153.618
Index ranges	$-11 \le h \le 11$ $-14 \le k \le 14$ $-20 \le l \le 20$	$-16 \le h \le 16$ $-40 \le k \le 40$ $-16 \le l \le 16$	$-14 \le h \le 15$ $-21 \le k \le 21$ $-21 \le l \le 21$	$-18 \le h \le 18$ $-11 \le k \le 11$ $-21 \le l \le 22$
Refl. collected	59098	64458	124304	29223
Independent refl.	6741	10143	14100	4967
R_{int}	0.0186	0.0418	0.0287	0.0477
Refl. with $I>2\sigma(I)$	6506	7019	13368	4818
Data / restraints / parameters	6741 / 221 / 426	10143 / 858 / 443	14100 / 0 / 631	4967 / 0 / 211
Goodness-of-Fit on F^2	1.023	1.035	1.033	1.058
R_1/wR_2 [$I > 2\sigma(I)$]	0.0320 / 0.0786	0.0657 / 0.1914	0.0255 / 0.0686	0.0337 / 0.0915
R_1/wR_2 (all data)	0.0329 / 0.0793	0.0936 / 0.2165	0.0269 /0.0696	0.0346 / 0.0940
ρ_{fin} (max/min) [e Å^{-3}]	0.67 / −0.61	0.66 / −0.52	0.36 / −0.31	0.38 / −0.39
CCDC	2151906	2151907	2151208	2151209

4) Computational details

All the calculations reported in this paper were performed with the Gaussian 09 suite of programs.[5] Electron correlation was partially taken into account using the metahybrid functional M06-2X[6] in conjunction with the standard double-ζ quality def2-SVP[7] basis set for all atoms. Solvent effects (solvent = *n*-hexane) were taken into account by means of the Polarization Continuum Model (PCM)[8] method. This level is denoted PCM(hexane)-M06-2X/def2-SVP. Geometries were fully optimized in solution without any geometry or symmetry constraints. Reactants, intermediates, and products were characterized by frequency calculations,[9] and have positive definite Hessian matrices. Transition structures (TS's) show only one negative eigenvalue in their diagonalized force constant matrices, and their associated eigenvectors were confirmed to correspond to the motion along the reaction coordinate under consideration using the Intrinsic Reaction Coordinate (IRC) method.[10] Frequency calculations were also used to determine the difference between the potential (E) and Gibbs (G) energies, G −E, which contains the zero-point, thermal, and entropy energies. Potential energies were refined, E_{sol}, by means of single point (SP) calculations at the same level with a larger basis set, def2-TZVPP,[7] where all elements were described with a triple-ζ plus polarization quality basis set. This level is denoted PCM(hexane)-M06-2X/def2-TZVPP//PCM(hexane)-M06-2X/def2-SVP. The Δ*G* and $\Delta G^{\neq}$ values given in the text were obtained from the Gibbs energy in solution, G_{sol}, which was calculated by adding the thermochemistry corrections, $G - E$, to the refined SP energies, E_{sol}, i.e., $G_{sol} = E_{sol} + G - E$

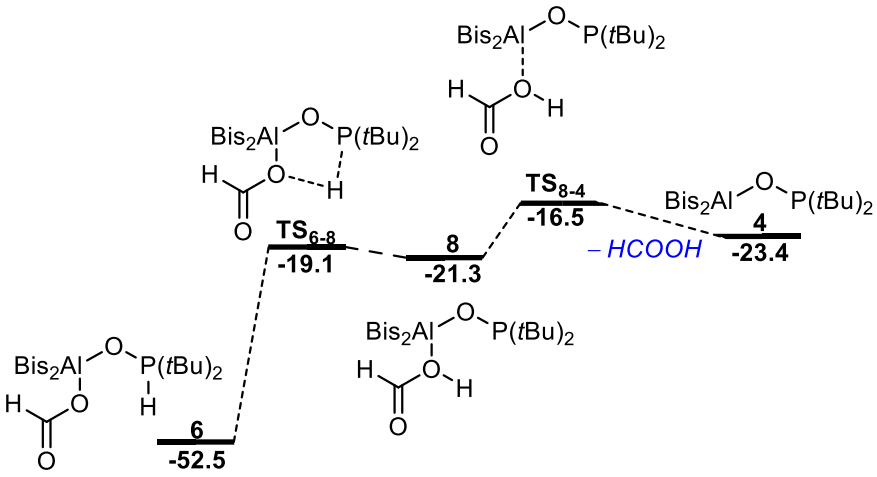

Figure S19. Computed reaction profile for the formation of formic acid from **6**. Relative free energies (at 298 K) and bond lengths are given in kcal/mol and Å, respectively. All data have been computed at the PCM(hexane-M06-2X/def2-TZVPP//PCM(hexane)-M06-2X/def2-SVP level.

Table S2. Cartesian coordinates (in Å) and free energies (in a.u.) of all the stationary points discussed in the text. All calculations have been performed at the PCM(*n*-hexane)-M06-2X/def2-TZVPP//PCM(*n*-hexane)-M06-2X/def2-SVP level.

CO_2: E= -188.6184995

C	0.000000000	0.000000000	0.000000000
O	0.000000000	0.000000000	-1.156152000
O	0.000000000	0.000000000	1.156152000

H_2: E= -1.1801616

H	0.000000000	0.000000000	0.377079000
H	0.000000000	0.000000000	-0.377079000

Formic acid: E= -189.7976676

H	1.044949000	-1.059991000	-0.000014000
H	-0.105418000	1.504927000	-0.000041000
C	-0.131375000	0.398138000	0.000016000
O	1.107085000	-0.090161000	-0.000001000
O	-1.125995000	-0.264060000	-0.000004000

1: E= -1957.5179354

Al	0.010138000	-0.090352000	-1.511096000
C	-1.810569000	-0.037129000	-0.781302000
H	-2.347914000	-0.066793000	-1.752588000
Si	-2.588520000	1.457345000	0.069781000
C	-1.736340000	3.078661000	-0.390895000
H	-2.314053000	3.927261000	0.008098000
H	-1.687102000	3.196687000	-1.485549000
H	-0.715848000	3.152911000	0.010903000
C	-2.636017000	1.316346000	1.954152000
H	-1.645609000	1.172815000	2.409028000
H	-3.278959000	0.483053000	2.275089000
H	-3.063277000	2.243136000	2.368261000
C	-4.372513000	1.615615000	-0.531933000
H	-4.967004000	0.722014000	-0.293142000
H	-4.399969000	1.760787000	-1.623052000
H	-4.860240000	2.484899000	-0.064161000
Si	-2.237713000	-1.698437000	-0.000868000
C	-1.251715000	-1.941533000	1.589520000
H	-1.691733000	-1.362914000	2.414698000
H	-0.211182000	-1.605629000	1.468170000
H	-1.233732000	-3.000785000	1.889271000
C	-1.831414000	-3.063014000	-1.248461000
H	-1.978553000	-4.058374000	-0.800775000
H	-0.799242000	-3.025926000	-1.630026000
H	-2.505405000	-2.979648000	-2.115509000
C	-4.072831000	-1.893402000	0.396408000
H	-4.425749000	-1.164860000	1.140799000
H	-4.251789000	-2.901693000	0.802088000
H	-4.686159000	-1.781768000	-0.510832000
C	1.825045000	0.039655000	-0.782902000
H	2.363490000	0.053948000	-1.753778000
Si	2.214794000	1.712683000	-0.018423000
C	4.044306000	1.934744000	0.395870000
H	4.398537000	1.216212000	1.149602000
H	4.209168000	2.948008000	0.795021000
H	4.668334000	1.822457000	-0.504085000
C	1.214080000	1.954142000	1.562516000
H	0.189709000	1.572146000	1.443127000
H	1.151292000	3.017636000	1.840109000

H	1.675333000	1.411885000	2.400804000
C	1.809658000	3.052698000	-1.291759000
H	2.511105000	2.975007000	-2.137372000
H	1.916437000	4.059010000	-0.857405000
H	0.789277000	2.977519000	-1.697893000
Si	2.615354000	-1.439663000	0.085230000
C	2.637185000	-1.280595000	1.967765000
H	3.271180000	-0.440639000	2.288893000
H	3.061804000	-2.200869000	2.398673000
H	1.638912000	-1.135877000	2.405066000
C	4.403476000	-1.594790000	-0.500801000
H	4.439473000	-1.754329000	-1.589572000
H	4.894806000	-2.453282000	-0.017221000
H	4.988093000	-0.692552000	-0.269920000
C	1.762543000	-3.064354000	-0.368202000
H	0.744025000	-3.136847000	0.040937000
H	2.339317000	-3.913546000	0.030746000
H	1.706355000	-3.186943000	-1.462247000
H	0.010921000	-0.308789000	-3.089957000

1d: E= -3915.072122

Al	1.323764000	0.000135000	-0.000042000
C	2.005007000	-1.839234000	-0.056271000
H	1.030392000	-2.366419000	-0.133428000
Si	2.745478000	-2.596608000	1.506692000
C	2.280084000	-1.629137000	3.060568000
H	2.581122000	-2.193517000	3.957186000
H	1.194320000	-1.456048000	3.121659000
H	2.786237000	-0.652829000	3.100155000
C	4.631720000	-2.711523000	1.465400000
H	5.110645000	-1.729901000	1.336198000
H	4.990841000	-3.370165000	0.661457000
H	4.984136000	-3.129724000	2.421356000
C	2.044586000	-4.340340000	1.699385000
H	2.319875000	-4.981342000	0.849088000
H	0.944381000	-4.310238000	1.756047000
H	2.417337000	-4.814082000	2.620559000
Si	2.863113000	-2.301036000	-1.665530000
C	4.446762000	-1.294297000	-1.863385000
H	5.228849000	-1.661919000	-1.182738000
H	4.273627000	-0.233614000	-1.626605000
H	4.835052000	-1.353612000	-2.891647000
C	1.681440000	-1.997791000	-3.110256000
H	2.190972000	-2.164983000	-4.072098000
H	1.255750000	-0.984179000	-3.125866000
H	0.845072000	-2.712976000	-3.048020000
C	3.294217000	-4.138554000	-1.767037000
H	3.986120000	-4.466718000	-0.978391000
H	3.769127000	-4.348600000	-2.738409000
H	2.383810000	-4.754707000	-1.701071000
C	2.004596000	1.839656000	0.056378000
H	1.029956000	2.366775000	0.133481000
Si	2.862759000	2.301305000	1.665651000
C	3.293773000	4.138836000	1.767400000
H	3.985793000	4.467071000	0.978889000
H	3.768574000	4.348798000	2.738848000
H	2.383366000	4.754985000	1.701400000
C	4.446527000	1.294585000	1.863069000
H	4.273922000	0.234385000	1.623726000
H	4.833658000	1.351657000	2.891898000
H	5.229280000	1.663911000	1.184121000

C	1.681354000	1.997754000	3.110500000
H	0.845303000	2.713356000	3.048954000
H	2.191246000	2.164141000	4.072291000
H	1.255210000	0.984324000	3.125613000
Si	2.745178000	2.597127000	-1.506511000
C	4.631425000	2.711749000	-1.465047000
H	4.990444000	3.371032000	-0.661582000
H	4.984068000	3.129155000	-2.421274000
H	5.110253000	1.730204000	-1.334927000
C	2.044610000	4.340993000	-1.699113000
H	0.944373000	4.311207000	-1.755351000
H	2.417139000	4.814553000	-2.620470000
H	2.320374000	4.981995000	-0.848972000
C	2.279618000	1.629790000	-3.060434000
H	2.786062000	0.653646000	-3.100351000
H	2.580212000	2.194361000	-3.957081000
H	1.193883000	1.456357000	-3.121239000
H	0.000057000	0.000206000	-1.141460000
Al	-1.323504000	-0.000087000	0.000064000
C	-2.004956000	1.839261000	-0.056113000
H	-1.030484000	2.366711000	-0.133042000
Si	-2.746005000	2.596331000	1.506763000
C	-2.280960000	1.628598000	3.060574000
H	-2.582489000	2.192625000	3.957253000
H	-1.195153000	1.455874000	3.121985000
H	-2.786823000	0.652126000	3.099734000
C	-4.632252000	2.711136000	1.464945000
H	-5.111096000	1.729472000	1.335757000
H	-4.991178000	3.369594000	0.660773000
H	-4.984972000	3.129486000	2.420720000
C	-2.045198000	4.340043000	1.699921000
H	-2.320084000	4.981096000	0.849529000
H	-0.945012000	4.309869000	1.756999000
H	-2.418279000	4.813773000	2.620961000
Si	-2.862830000	2.301083000	-1.665493000
C	-4.446522000	1.294423000	-1.863618000
H	-5.229323000	1.663555000	-1.184612000
H	-4.274091000	0.234098000	-1.624746000
H	-4.833485000	1.352065000	-2.892477000
C	-1.680929000	1.998116000	-3.110075000
H	-2.190396000	2.165255000	-4.071961000
H	-1.255073000	0.984573000	-3.125697000
H	-0.844695000	2.713454000	-3.047727000
C	-3.294059000	4.138599000	-1.766959000
H	-3.985845000	4.466761000	-0.978222000
H	-3.769182000	4.348545000	-2.738255000
H	-2.383704000	4.754854000	-1.701244000
C	-2.004505000	-1.839605000	0.056234000
H	-1.029957000	-2.366879000	0.133485000
Si	-2.862809000	-2.301467000	1.665343000
C	-3.293741000	-4.139051000	1.766758000
H	-3.985382000	-4.467224000	0.977886000
H	-3.768985000	-4.349155000	2.737958000
H	-2.383299000	-4.755186000	1.701092000
C	-4.446768000	-1.295110000	1.862867000
H	-4.274609000	-0.234961000	1.622981000
H	-4.833579000	-1.351900000	2.891828000
H	-5.229573000	-1.665026000	1.184293000
C	-1.681376000	-1.998116000	3.110233000
H	-0.845127000	-2.713457000	3.048305000
H	-2.191097000	-2.164980000	4.072030000

H	-1.255503000	-0.984579000	3.125653000
Si	-2.744954000	-2.596703000	-1.506887000
C	-4.631179000	-2.711830000	-1.465540000
H	-4.990115000	-3.370862000	-0.661838000
H	-4.983710000	-3.129600000	-2.421637000
H	-5.110180000	-1.730319000	-1.335736000
C	-2.043830000	-4.340311000	-1.699907000
H	-0.943610000	-4.310091000	-1.756154000
H	-2.416221000	-4.813920000	-2.621290000
H	-2.319353000	-4.981487000	-0.849812000
C	-2.279652000	-1.628764000	-3.060512000
H	-2.785812000	-0.652445000	-3.099776000
H	-2.580749000	-2.192781000	-3.957339000
H	-1.193881000	-1.455667000	-3.121588000
H	0.000125000	-0.000141000	1.141523000

2: E= -732.9070525

P	-0.000945000	0.651503000	-0.421540000
H	0.012118000	0.539579000	-1.845525000
O	-0.027538000	2.055411000	0.112259000
C	1.569783000	-0.232485000	0.014290000
C	2.671442000	0.795308000	-0.290366000
H	2.693654000	1.054301000	-1.360685000
H	3.650098000	0.366426000	-0.024175000
H	2.511211000	1.719540000	0.279794000
C	1.584700000	-0.565435000	1.509328000
H	1.327773000	0.319022000	2.111402000
H	2.593336000	-0.897308000	1.801712000
H	0.882940000	-1.375910000	1.755577000
C	1.793982000	-1.484848000	-0.836229000
H	1.084043000	-2.288173000	-0.602242000
H	2.807830000	-1.871412000	-0.645534000
H	1.723599000	-1.261657000	-1.912148000
C	-1.562886000	-0.247058000	0.012184000
C	-1.860627000	-0.003990000	1.496290000
H	-1.141957000	-0.515494000	2.151257000
H	-2.866074000	-0.385997000	1.732771000
H	-1.827813000	1.071153000	1.719949000
C	-1.527903000	-1.739430000	-0.312714000
H	-1.221837000	-1.927910000	-1.353785000
H	-2.537534000	-2.160895000	-0.183139000
H	-0.852240000	-2.291379000	0.356498000
C	-2.642497000	0.449350000	-0.832592000
H	-2.621557000	1.536355000	-0.668325000
H	-3.634989000	0.070963000	-0.542562000
H	-2.504087000	0.254487000	-1.906952000

3a: E= -2690.4648005

P	-2.685669000	-0.463542000	0.342343000
H	-2.711046000	-1.506748000	1.298613000
Si	2.113875000	-2.679558000	-1.290835000
Si	1.023039000	-2.282035000	1.662416000
Si	2.836668000	2.056683000	0.672210000
Si	0.401468000	3.229869000	-0.924828000
Al	0.543068000	0.061051000	-0.592368000
O	-1.235550000	-0.116302000	-0.008315000
C	1.617165000	-1.499046000	0.077511000
H	2.569474000	-1.008581000	0.361751000
C	1.047109000	1.851036000	0.166026000
H	0.466843000	1.900162000	1.110238000
C	0.636367000	-3.348593000	-2.262912000

H	-0.070773000	-3.895379000	-1.621019000
H	0.991883000	-4.043626000	-3.039838000
H	0.101119000	-2.527425000	-2.763462000
C	3.073455000	-4.192658000	-0.665128000
H	3.971173000	-3.889503000	-0.103789000
H	3.399865000	-4.808057000	-1.518504000
H	2.463462000	-4.830894000	-0.006954000
C	3.252020000	-1.816764000	-2.529409000
H	2.800627000	-0.888967000	-2.913201000
H	3.453722000	-2.480484000	-3.384975000
H	4.219589000	-1.564014000	-2.068382000
C	-0.255653000	-3.639947000	1.327677000
H	-1.074296000	-3.260744000	0.696919000
H	-0.689072000	-4.010469000	2.269764000
H	0.194978000	-4.496161000	0.802527000
C	0.194632000	-1.031774000	2.824898000
H	0.801845000	-0.119131000	2.923413000
H	0.053281000	-1.463948000	3.827702000
H	-0.788613000	-0.734834000	2.436283000
C	2.434949000	-3.048385000	2.662367000
H	2.962484000	-3.826562000	2.093645000
H	2.048696000	-3.501069000	3.589250000
H	3.172299000	-2.281832000	2.947911000
C	3.228195000	1.110791000	2.267989000
H	2.594528000	1.471892000	3.093861000
H	4.277563000	1.286538000	2.552921000
H	3.080868000	0.025312000	2.178281000
C	4.013341000	1.462755000	-0.682239000
H	3.827469000	0.410063000	-0.941880000
H	5.059964000	1.551759000	-0.351780000
H	3.896879000	2.055402000	-1.601539000
C	3.310689000	3.848900000	1.083101000
H	3.183833000	4.535223000	0.232800000
H	4.367096000	3.890308000	1.392810000
H	2.701680000	4.229893000	1.918183000
C	1.617600000	3.682105000	-2.300016000
H	2.564357000	4.095178000	-1.921801000
H	1.163268000	4.431611000	-2.966755000
H	1.849500000	2.789803000	-2.903013000
C	-0.001512000	4.788634000	0.076503000
H	-0.779945000	4.578954000	0.827602000
H	-0.378259000	5.585081000	-0.584562000
H	0.881453000	5.172029000	0.607112000
C	-1.206941000	2.747135000	-1.813884000
H	-0.983990000	2.174489000	-2.726341000
H	-1.794671000	3.636602000	-2.090520000
H	-1.822956000	2.101912000	-1.172949000
C	-3.553411000	0.928670000	1.210930000
C	-2.469697000	1.740218000	1.934734000
H	-1.893323000	1.128942000	2.644135000
H	-2.958785000	2.549720000	2.497343000
H	-1.764681000	2.185396000	1.218745000
C	-4.327930000	1.857563000	0.265918000
H	-3.676824000	2.334324000	-0.478018000
H	-4.776138000	2.658251000	0.873472000
H	-5.145351000	1.343743000	-0.256385000
C	-4.518196000	0.304121000	2.230607000
H	-5.288945000	-0.316003000	1.749946000
H	-5.031060000	1.114777000	2.769502000
H	-3.986891000	-0.309309000	2.972826000
C	-3.546077000	-1.178011000	-1.117959000

C	-3.398724000	-0.219711000	-2.306273000
H	-3.921945000	0.732731000	-2.148951000
H	-3.829705000	-0.700059000	-3.197697000
H	-2.337797000	-0.008058000	-2.508159000
C	-5.010935000	-1.497708000	-0.803859000
H	-5.107404000	-2.152513000	0.076091000
H	-5.438820000	-2.038021000	-1.661894000
H	-5.620480000	-0.598744000	-0.642820000
C	-2.792059000	-2.480015000	-1.424640000
H	-1.716179000	-2.300171000	-1.554299000
H	-3.179000000	-2.899400000	-2.365616000
H	-2.935338000	-3.232733000	-0.634705000
H	0.375019000	0.047911000	-2.198808000

3b: E= -4372.8694826

P	-2.773785000	-0.399219000	0.349999000
H	-2.831311000	-1.446379000	1.304351000
Si	2.046308000	-2.807400000	-1.204227000
Si	0.897677000	-2.286712000	1.719814000
Si	2.900579000	2.004308000	0.703220000
Si	0.465221000	3.252371000	-0.860498000
Ga	0.624459000	0.047698000	-0.607398000
O	-1.326996000	-0.054954000	0.005346000
C	1.601214000	-1.579123000	0.140931000
H	2.574498000	-1.148602000	0.447081000
C	1.099229000	1.849900000	0.209726000
H	0.517150000	1.878173000	1.152197000
C	0.544363000	-3.391935000	-2.191744000
H	-0.197720000	-3.896494000	-1.554788000
H	0.866500000	-4.106516000	-2.965440000
H	0.058502000	-2.543746000	-2.697354000
C	2.901905000	-4.363119000	-0.539323000
H	3.792943000	-4.105495000	0.054249000
H	3.225907000	-4.999138000	-1.378312000
H	2.233869000	-4.964432000	0.096892000
C	3.250517000	-2.011162000	-2.424748000
H	2.840392000	-1.078640000	-2.842444000
H	3.460320000	-2.696384000	-3.260980000
H	4.208792000	-1.775064000	-1.936073000
C	-0.471752000	-3.541260000	1.348692000
H	-1.206823000	-3.122377000	0.645592000
H	-0.999478000	-3.835133000	2.269494000
H	-0.060184000	-4.453155000	0.888481000
C	0.162860000	-0.951858000	2.843461000
H	0.935698000	-0.233126000	3.154704000
H	-0.272387000	-1.400258000	3.750409000
H	-0.616451000	-0.388332000	2.313949000
C	2.216608000	-3.155081000	2.762352000
H	2.660477000	-4.014047000	2.240219000
H	1.780380000	-3.516135000	3.707212000
H	3.029500000	-2.456264000	3.015416000
C	3.285205000	1.040297000	2.288496000
H	2.677339000	1.420994000	3.124693000
H	4.344512000	1.179174000	2.556333000
H	3.098348000	-0.039112000	2.198391000
C	4.033794000	1.377237000	-0.674138000
H	3.828236000	0.323266000	-0.916417000
H	5.090326000	1.453810000	-0.373665000
H	3.900523000	1.961665000	-1.596566000
C	3.425350000	3.781766000	1.108868000
H	3.299977000	4.472858000	0.262460000

H	4.488005000	3.795038000	1.398962000
H	2.841936000	4.175568000	1.956099000
C	1.675267000	3.690769000	-2.246370000
H	2.637540000	4.074440000	-1.876460000
H	1.231313000	4.461418000	-2.895740000
H	1.876532000	2.803356000	-2.867404000
C	0.113577000	4.804024000	0.167515000
H	-0.666131000	4.602330000	0.919280000
H	-0.244067000	5.622395000	-0.476960000
H	1.009908000	5.153319000	0.699299000
C	-1.161590000	2.805961000	-1.727370000
H	-0.969058000	2.178612000	-2.610617000
H	-1.702970000	3.709031000	-2.049973000
H	-1.805869000	2.226413000	-1.052679000
C	-3.648242000	0.990903000	1.220528000
C	-2.569502000	1.771520000	1.984450000
H	-2.045777000	1.141492000	2.717665000
H	-3.052766000	2.597745000	2.527699000
H	-1.820493000	2.189536000	1.296849000
C	-4.381350000	1.946306000	0.269423000
H	-3.706095000	2.409285000	-0.462057000
H	-4.820284000	2.755700000	0.872453000
H	-5.201930000	1.455198000	-0.269767000
C	-4.648717000	0.374112000	2.209164000
H	-5.422231000	-0.221721000	1.703608000
H	-5.155021000	1.187383000	2.750812000
H	-4.146961000	-0.262840000	2.952101000
C	-3.647638000	-1.094025000	-1.116677000
C	-3.483807000	-0.129105000	-2.297491000
H	-4.000203000	0.826588000	-2.138240000
H	-3.910040000	-0.598664000	-3.197060000
H	-2.419864000	0.076544000	-2.487403000
C	-5.118021000	-1.395700000	-0.812998000
H	-5.227261000	-2.055878000	0.061478000
H	-5.551718000	-1.921951000	-1.677049000
H	-5.714596000	-0.489090000	-0.645670000
C	-2.913495000	-2.403878000	-1.436936000
H	-1.835524000	-2.237011000	-1.568286000
H	-3.309527000	-2.812049000	-2.379286000
H	-3.063350000	-3.160086000	-0.651597000
H	0.399532000	0.020840000	-2.204723000

3c: E= -2638.0699590

P	2.981446000	0.061961000	0.311710000
H	3.142355000	1.191726000	1.154683000
Si	-1.643270000	3.193398000	-1.095253000
Si	-0.507817000	2.417354000	1.791750000
Si	-3.284237000	-1.637271000	0.691736000
Si	-0.991186000	-3.382522000	-0.645358000
In	-0.618875000	-0.036463000	-0.628178000
O	1.509217000	-0.278077000	0.096690000
C	-1.370321000	1.892375000	0.220684000
H	-2.387877000	1.590617000	0.537670000
C	-1.460730000	-1.865796000	0.338490000
H	-0.932117000	-1.924738000	1.310080000
C	-0.091321000	3.552596000	-2.115298000
H	0.759291000	3.859738000	-1.488556000
H	-0.299095000	4.368480000	-2.825371000
H	0.204713000	2.667727000	-2.699747000
C	-2.231911000	4.850215000	-0.388559000
H	-3.147592000	4.724992000	0.209878000

H	-2.454987000	5.552692000	-1.207022000
H	-1.468199000	5.315610000	0.253857000
C	-2.972110000	2.606830000	-2.306106000
H	-2.684963000	1.657880000	-2.786930000
H	-3.127130000	3.352653000	-3.101398000
H	-3.936674000	2.452673000	-1.797890000
C	1.045202000	3.424454000	1.387625000
H	1.657963000	2.908687000	0.632886000
H	1.661982000	3.586094000	2.285403000
H	0.782229000	4.412210000	0.977267000
C	0.001828000	0.931784000	2.850587000
H	-0.887482000	0.363553000	3.165393000
H	0.532378000	1.260155000	3.758713000
H	0.651719000	0.246415000	2.287330000
C	-1.624277000	3.473735000	2.896015000
H	-1.943275000	4.399709000	2.397299000
H	-1.100282000	3.746847000	3.825627000
H	-2.529085000	2.910734000	3.174802000
C	-3.545746000	-0.597787000	2.251218000
H	-3.087890000	-1.094286000	3.121490000
H	-4.620497000	-0.478262000	2.458576000
H	-3.104298000	0.406165000	2.165688000
C	-4.133993000	-0.777120000	-0.766034000
H	-3.726733000	0.232301000	-0.937327000
H	-5.214743000	-0.669692000	-0.584876000
H	-4.003403000	-1.352263000	-1.695948000
C	-4.223694000	-3.255020000	0.997943000
H	-4.202597000	-3.922169000	0.122825000
H	-5.278516000	-3.034555000	1.226089000
H	-3.799864000	-3.803169000	1.853625000
C	-2.016635000	-3.511051000	-2.227392000
H	-3.086858000	-3.653859000	-2.013244000
H	-1.679810000	-4.363086000	-2.837681000
H	-1.908635000	-2.597025000	-2.832923000
C	-1.188572000	-4.983395000	0.346655000
H	-0.580582000	-4.944059000	1.264384000
H	-0.848695000	-5.847464000	-0.246023000
H	-2.232067000	-5.161452000	0.641416000
C	0.835661000	-3.310641000	-1.137015000
H	1.031539000	-2.501958000	-1.858017000
H	1.174554000	-4.261214000	-1.577185000
H	1.432533000	-3.107346000	-0.235636000
C	3.856661000	-1.264208000	1.257888000
C	2.835041000	-1.780593000	2.283856000
H	2.492754000	-0.979676000	2.956720000
H	3.315303000	-2.557971000	2.897051000
H	1.951207000	-2.209902000	1.792058000
C	4.313179000	-2.415890000	0.354529000
H	3.489250000	-2.817457000	-0.251381000
H	4.691359000	-3.230627000	0.990987000
H	5.129770000	-2.116273000	-0.317395000
C	5.056456000	-0.657345000	1.997484000
H	5.823105000	-0.269287000	1.313655000
H	5.524320000	-1.443458000	2.609599000
H	4.749731000	0.152750000	2.675529000
C	3.768654000	0.576290000	-1.274944000
C	3.442438000	-0.464268000	-2.353281000
H	3.889266000	-1.445084000	-2.142934000
H	3.842410000	-0.109472000	-3.315569000
H	2.354570000	-0.586444000	-2.459881000
C	5.276787000	0.790899000	-1.129855000

H	5.515120000	1.497283000	-0.319733000
H	5.660513000	1.222360000	-2.067039000
H	5.819004000	-0.147750000	-0.951980000
C	3.090586000	1.903862000	-1.642723000
H	1.996908000	1.798845000	-1.677809000
H	3.427513000	2.215066000	-2.643386000
H	3.347020000	2.706798000	-0.934879000
H	-0.254958000	-0.081848000	-2.372102000

4a: E= -2689.2821577

P	0.933852000	2.491862000	-0.849807000
Si	-2.906014000	-0.725608000	1.704675000
Al	-0.177617000	-0.483506000	0.016097000
O	0.641200000	1.012759000	-0.165792000
C	-0.053855000	3.603756000	0.318519000
C	-1.501416000	3.144550000	0.104214000
H	-1.643178000	2.090544000	0.385547000
H	-2.183143000	3.749194000	0.726018000
H	-1.803769000	3.263808000	-0.948187000
C	0.041818000	5.060529000	-0.149607000
H	1.020043000	5.510643000	0.058982000
H	-0.152139000	5.143633000	-1.230644000
H	-0.719145000	5.661819000	0.374254000
C	0.306515000	3.473937000	1.796300000
H	1.252961000	3.982382000	2.028452000
H	-0.478314000	3.934205000	2.420143000
H	0.398217000	2.416060000	2.090910000
C	2.776089000	2.661160000	-0.449674000
C	3.448877000	1.839689000	-1.561191000
H	3.250398000	2.271600000	-2.553556000
H	4.539748000	1.813590000	-1.403947000
H	3.079542000	0.803347000	-1.565391000
C	3.193525000	2.087735000	0.903092000
H	2.790362000	1.076219000	1.036622000
H	4.293838000	2.024132000	0.953543000
H	2.857425000	2.704682000	1.745676000
C	3.219607000	4.120046000	-0.576690000
H	2.808708000	4.599695000	-1.480129000
H	2.922205000	4.712639000	0.299998000
H	4.318693000	4.164311000	-0.647670000
C	0.878045000	-2.106075000	0.232224000
C	2.200608000	-4.467195000	-1.358769000
H	1.697737000	-5.204104000	-0.713868000
H	2.307193000	-4.909563000	-2.361380000
H	3.210318000	-4.297454000	-0.955908000
C	2.095408000	-1.651064000	-2.589253000
H	2.190571000	-2.072075000	-3.602136000
H	1.546662000	-0.697861000	-2.674850000
H	3.107346000	-1.422944000	-2.223327000
C	1.969990000	-0.800551000	2.835545000
H	2.897428000	-0.522680000	3.360466000
H	1.496027000	0.133246000	2.491821000
C	2.606990000	-3.693812000	2.233782000
H	3.430282000	-3.639730000	2.963074000
H	1.700458000	-4.011814000	2.772433000
H	2.855196000	-4.470265000	1.495750000
H	-1.741572000	-2.815208000	2.460625000
H	-5.324595000	-0.915305000	1.017710000
C	-3.022662000	0.992079000	2.472156000
H	-3.498361000	0.915597000	3.462294000
H	-2.026265000	1.440435000	2.610196000

H	-3.621745000	1.679218000	1.857302000
C	-4.130609000	-1.414924000	-2.183744000
H	-4.717809000	-1.055111000	-3.042847000
H	-4.831219000	-1.821794000	-1.438491000
C	-1.943683000	0.632866000	-2.782244000
H	-2.516099000	1.038471000	-3.630861000
H	-1.274997000	1.428354000	-2.416661000
H	-1.309238000	-0.179028000	-3.175592000
Si	1.202625000	-2.868854000	-1.457251000
Si	2.332282000	-2.011570000	1.420396000
Si	-3.100995000	-0.018137000	-1.437310000
H	0.150939000	-2.795099000	0.708333000
C	-0.458389000	-3.279743000	-2.264453000
H	-0.306273000	-3.790403000	-3.227751000
H	-1.064584000	-3.939322000	-1.623387000
H	-1.049512000	-2.371208000	-2.463327000
H	1.303542000	-1.272195000	3.574097000
C	3.935585000	-1.520295000	0.552425000
H	3.844683000	-0.582027000	-0.012121000
H	4.733415000	-1.386799000	1.299861000
H	4.260545000	-2.307500000	-0.145321000
C	-2.108940000	-0.734887000	0.000564000
C	-1.855218000	-1.794452000	2.859131000
H	-0.846544000	-1.371262000	2.993334000
H	-2.317503000	-1.869932000	3.855337000
C	-4.629384000	-1.495869000	1.642372000
H	-5.058788000	-1.559381000	2.654251000
H	-4.580073000	-2.516852000	1.232595000
C	-4.315334000	1.340880000	-0.942024000
H	-4.860481000	1.672919000	-1.839570000
H	-5.059987000	0.965323000	-0.223756000
H	-3.829362000	2.220139000	-0.499837000
H	-3.491074000	-2.240567000	-2.531783000
H	-2.099043000	-1.824956000	-0.216329000

4b: E= -4371.676467

P	0.920311000	2.495736000	-0.812927000
Si	-2.947003000	-0.722618000	1.701403000
Ga	-0.181321000	-0.520692000	0.044873000
O	0.720754000	1.052895000	-0.032217000
C	-0.097254000	3.639684000	0.300266000
C	-1.529802000	3.128763000	0.103269000
H	-1.637995000	2.077263000	0.409242000
H	-2.231072000	3.724952000	0.711667000
H	-1.835952000	3.213282000	-0.951230000
C	-0.048755000	5.076630000	-0.231242000
H	0.903298000	5.577347000	-0.018260000
H	-0.215983000	5.103182000	-1.319815000
H	-0.848100000	5.668730000	0.244180000
C	0.264827000	3.584385000	1.782196000
H	1.202580000	4.119183000	1.990159000
H	-0.527632000	4.059297000	2.385448000
H	0.376637000	2.542551000	2.122880000
C	2.759308000	2.774708000	-0.451510000
C	3.457395000	1.961606000	-1.553530000
H	3.236767000	2.371142000	-2.550730000
H	4.549573000	1.977558000	-1.403283000
H	3.125383000	0.912727000	-1.542061000
C	3.222139000	2.257008000	0.909989000
H	2.898690000	1.219921000	1.062287000
H	4.324059000	2.284824000	0.959264000

H	2.835972000	2.859504000	1.741851000
C	3.133904000	4.248613000	-0.618625000
H	2.687380000	4.688887000	-1.525160000
H	2.824428000	4.847437000	0.249712000
H	4.228886000	4.339891000	-0.709362000
C	0.947402000	-2.132935000	0.248836000
C	2.352543000	-4.403110000	-1.383407000
H	1.883679000	-5.164998000	-0.741832000
H	2.473734000	-4.833403000	-2.389495000
H	3.355551000	-4.193371000	-0.982660000
C	2.117867000	-1.569118000	-2.572425000
H	2.215627000	-1.959518000	-3.597184000
H	1.530516000	-0.636516000	-2.625757000
H	3.124088000	-1.309393000	-2.212588000
C	1.995356000	-0.743874000	2.816285000
H	2.899081000	-0.470426000	3.383047000
H	1.551226000	0.187794000	2.429211000
C	2.756211000	-3.627862000	2.237980000
H	3.587552000	-3.542863000	2.954935000
H	1.870471000	-3.980198000	2.789507000
H	3.023136000	-4.394416000	1.495732000
H	-1.774296000	-2.803477000	2.465644000
H	-5.356283000	-0.919755000	0.988938000
C	-3.071559000	0.997693000	2.457898000
H	-3.558469000	0.922636000	3.442720000
H	-2.076577000	1.445251000	2.606467000
H	-3.663959000	1.682921000	1.834798000
C	-4.129584000	-1.423393000	-2.215259000
H	-4.706924000	-1.066652000	-3.082236000
H	-4.838912000	-1.830238000	-1.478144000
C	-1.921457000	0.610270000	-2.783978000
H	-2.470350000	1.044546000	-3.633879000
H	-1.230258000	1.379458000	-2.402901000
H	-1.311398000	-0.219060000	-3.179362000
Si	1.288490000	-2.847839000	-1.461145000
Si	2.408276000	-1.959752000	1.425299000
Si	-3.109680000	-0.024247000	-1.460919000
H	0.257037000	-2.860151000	0.720372000
C	-0.364806000	-3.309839000	-2.254991000
H	-0.209349000	-3.789876000	-3.233302000
H	-0.932624000	-4.008789000	-1.620813000
H	-0.995738000	-2.421325000	-2.420486000
H	1.287067000	-1.200387000	3.525086000
C	3.976098000	-1.400955000	0.537162000
H	3.828654000	-0.465485000	-0.019891000
H	4.777260000	-1.231170000	1.273498000
H	4.328466000	-2.167968000	-0.169614000
C	-2.146054000	-0.752915000	-0.005637000
C	-1.895430000	-1.782778000	2.861791000
H	-0.889926000	-1.352142000	2.998439000
H	-2.359788000	-1.859088000	3.856878000
C	-4.665918000	-1.498911000	1.620222000
H	-5.105254000	-1.563515000	2.627740000
H	-4.609565000	-2.519683000	1.211012000
C	-4.326610000	1.334780000	-0.977130000
H	-4.856659000	1.675924000	-1.880185000
H	-5.083031000	0.954753000	-0.273688000
H	-3.844822000	2.208198000	-0.519552000
H	-3.483833000	-2.248216000	-2.554222000
H	-2.157875000	-1.843135000	-0.216350000

4c: E= -2636.8671433

P	0.421240000	2.708121000	-0.798795000
Si	-2.998271000	-1.253040000	1.690178000
In	-0.084482000	-0.633712000	0.079344000
O	0.519125000	1.313147000	0.060771000
C	-0.885772000	3.648650000	0.206044000
C	-2.158049000	2.824053000	-0.030007000
H	-2.048439000	1.784152000	0.315571000
H	-3.005540000	3.268032000	0.520298000
H	-2.419277000	2.804449000	-1.100015000
C	-1.131195000	5.039417000	-0.388619000
H	-0.337039000	5.753312000	-0.140030000
H	-1.220082000	4.991738000	-1.485978000
H	-2.077164000	5.447025000	0.005528000
C	-0.598712000	3.726943000	1.703058000
H	0.189360000	4.461393000	1.923913000
H	-1.504064000	4.037451000	2.252411000
H	-0.279256000	2.746815000	2.091945000
C	2.131849000	3.430638000	-0.401503000
C	3.037291000	2.779823000	-1.459384000
H	2.763619000	3.107285000	-2.473613000
H	4.091558000	3.047951000	-1.277291000
H	2.953460000	1.682705000	-1.430627000
C	2.652437000	3.060757000	0.986760000
H	2.586525000	1.977238000	1.150619000
H	3.710598000	3.361128000	1.076484000
H	2.093745000	3.559836000	1.789255000
C	2.159011000	4.946622000	-0.598653000
H	1.653660000	5.249446000	-1.530314000
H	1.684202000	5.472569000	0.241773000
H	3.204160000	5.293217000	-0.658623000
C	1.581465000	-2.020795000	0.270887000
C	3.568616000	-3.736599000	-1.423622000
H	3.333104000	-4.628948000	-0.823304000
H	3.818013000	-4.068952000	-2.443121000
H	4.465110000	-3.265321000	-0.993319000
C	2.534617000	-1.047005000	-2.512137000
H	2.753276000	-1.353400000	-3.546679000
H	1.710461000	-0.313650000	-2.552922000
H	3.420409000	-0.525267000	-2.121099000
C	2.094272000	-0.386954000	2.833663000
H	2.843356000	0.020241000	3.530567000
H	1.540454000	0.467541000	2.407250000
C	3.704805000	-2.928263000	2.296182000
H	4.481014000	-2.613386000	3.010513000
H	2.957459000	-3.520380000	2.846612000
H	4.174628000	-3.584036000	1.548116000
H	-1.445974000	-3.018770000	2.579282000
H	-5.303925000	-1.896106000	0.930171000
C	-3.428788000	0.462932000	2.335458000
H	-3.934899000	0.361557000	3.308386000
H	-2.528414000	1.077972000	2.488891000
H	-4.101174000	1.007986000	1.657769000
C	-3.837678000	-2.222376000	-2.355683000
H	-4.406766000	-1.953274000	-3.258846000
H	-4.517864000	-2.750162000	-1.669432000
C	-1.916966000	0.121398000	-2.749792000
H	-2.434814000	0.461944000	-3.659812000
H	-1.395583000	0.995533000	-2.322947000
H	-1.152417000	-0.607784000	-3.070700000
Si	2.102754000	-2.549692000	-1.454835000

Si	2.899665000	-1.430603000	1.477105000
Si	-3.113063000	-0.687396000	-1.529008000
H	1.104917000	-2.907805000	0.732746000
C	0.641627000	-3.440010000	-2.264726000
H	0.901056000	-3.788900000	-3.275961000
H	0.339756000	-4.317104000	-1.671047000
H	-0.240071000	-2.783555000	-2.359488000
H	1.396031000	-1.003013000	3.422698000
C	4.245766000	-0.420795000	0.626879000
H	3.834139000	0.445206000	0.089283000
H	4.954253000	-0.040641000	1.379515000
H	4.815268000	-1.031889000	-0.090336000
C	-2.167527000	-1.256297000	0.003022000
C	-1.796364000	-2.033691000	2.926198000
H	-0.911366000	-1.391175000	3.074868000
H	-2.265021000	-2.169819000	3.912863000
C	-4.561156000	-2.309158000	1.629320000
H	-5.030633000	-2.369965000	2.623236000
H	-4.323227000	-3.333204000	1.302259000
C	-4.549188000	0.476400000	-1.153821000
H	-5.062641000	0.727927000	-2.095022000
H	-5.286029000	-0.006031000	-0.493179000
H	-4.230871000	1.415309000	-0.682222000
H	-3.042969000	-2.924486000	-2.652040000
H	-1.997412000	-2.338966000	-0.172261000

5: E= -2877.9370930

P	0.627567000	-2.344179000	0.040288000
Si	1.546462000	2.365706000	1.826581000
Al	-0.112298000	0.483318000	-0.133938000
O	0.306119000	-1.046957000	0.858856000
O	0.106204000	-0.491312000	-1.718355000
O	0.645019000	-2.450012000	-2.684839000
C	0.460194000	-1.725463000	-1.738694000
C	2.370980000	-2.864505000	0.328437000
C	3.183144000	-1.581061000	0.104801000
H	2.874293000	-0.781284000	0.790394000
H	4.247006000	-1.800320000	0.282426000
H	3.088127000	-1.214092000	-0.929027000
C	2.812623000	-3.931618000	-0.681708000
H	2.348682000	-4.906297000	-0.489359000
H	2.587710000	-3.633805000	-1.715281000
H	3.901948000	-4.056942000	-0.586007000
C	2.546965000	-3.353167000	1.770399000
H	2.069691000	-4.330373000	1.930305000
H	3.622641000	-3.472101000	1.970666000
H	2.144248000	-2.632374000	2.497600000
C	-0.707845000	-3.584540000	0.297640000
C	-1.957851000	-2.928518000	-0.311498000
H	-1.890441000	-2.864636000	-1.407564000
H	-2.837572000	-3.539820000	-0.058911000
H	-2.121257000	-1.917173000	0.092852000
C	-0.926010000	-3.814643000	1.797409000
H	-1.144165000	-2.871642000	2.316214000
H	-1.792024000	-4.482546000	1.922605000
H	-0.062763000	-4.293136000	2.277741000
C	-0.391136000	-4.890667000	-0.437267000
H	-0.077064000	-4.705336000	-1.475518000
H	0.386930000	-5.469608000	0.078640000
H	-1.303542000	-5.505768000	-0.459219000
C	-1.970811000	1.128522000	0.013034000

C	-4.237122000	2.484483000	-1.653192000
H	-4.009008000	3.451904000	-1.178592000
H	-4.595521000	2.686204000	-2.674774000
H	-5.062681000	2.021238000	-1.092610000
C	-3.115986000	-0.231708000	-2.570393000
H	-3.623469000	-0.026609000	-3.525873000
H	-2.195604000	-0.792448000	-2.791726000
H	-3.780086000	-0.864883000	-1.963854000
C	-2.421305000	-0.416188000	2.749601000
H	-2.409162000	0.188958000	3.669202000
H	-3.002311000	-1.327200000	2.963876000
C	-4.008288000	2.101546000	2.077686000
H	-4.751672000	1.819021000	2.839221000
H	-3.246023000	2.729820000	2.564480000
H	-4.513472000	2.708817000	1.311599000
H	-0.719080000	3.337536000	2.297198000
H	3.452325000	4.012095000	1.562498000
C	2.524399000	1.018204000	2.720323000
H	2.665196000	1.292828000	3.777047000
H	1.966873000	0.069079000	2.684094000
H	3.518184000	0.860827000	2.275859000
C	2.749117000	3.934060000	-1.681159000
H	3.604389000	4.113456000	-2.350989000
H	2.838424000	4.613798000	-0.820789000
C	2.564412000	1.121098000	-2.735160000
H	3.416154000	1.389927000	-3.380203000
H	2.579037000	0.031264000	-2.592744000
H	1.639293000	1.358113000	-3.280765000
Si	-2.690772000	1.392047000	-1.706266000
Si	-3.205340000	0.567911000	1.318068000
Si	2.679417000	2.123641000	-1.135611000
H	-1.757864000	2.168417000	0.339255000
C	-1.422471000	2.306055000	-2.772374000
H	-1.834236000	2.517870000	-3.771234000
H	-1.136785000	3.266564000	-2.314138000
H	-0.513871000	1.698658000	-2.906586000
H	-1.385445000	-0.710920000	2.526523000
C	-4.623520000	-0.497572000	0.647076000
H	-4.290660000	-1.472442000	0.263983000
H	-5.326850000	-0.688468000	1.473149000
H	-5.180531000	0.007867000	-0.155501000
C	1.211991000	1.932436000	0.030436000
C	-0.091562000	2.556836000	2.755779000
H	-0.668816000	1.619206000	2.765435000
H	0.095384000	2.844391000	3.802266000
C	2.454450000	4.014112000	2.025304000
H	2.579496000	4.247606000	3.094192000
H	1.872936000	4.830113000	1.568138000
C	4.355750000	1.727583000	-0.345457000
H	5.146279000	1.928011000	-1.085714000
H	4.554275000	2.360345000	0.532163000
H	4.453155000	0.678724000	-0.033424000
H	1.831063000	4.200076000	-2.228938000
H	0.558399000	2.771304000	-0.293667000

6: E= -2879.1270990

P	-2.705470000	0.200639000	-0.470700000
H	-2.785298000	1.287832000	-1.369823000
Si	1.715929000	2.892416000	1.169909000
Si	0.651834000	2.510710000	-1.789091000
Si	3.063675000	-1.612578000	-1.030253000

Si	0.809155000	-3.155569000	0.525674000
Al	0.590412000	-0.010821000	0.247890000
O	-1.263431000	0.073140000	0.056003000
C	1.398817000	1.726538000	-0.269762000
H	2.414448000	1.423736000	-0.592972000
C	1.243410000	-1.688078000	-0.577040000
H	0.720838000	-1.838233000	-1.540283000
C	0.145247000	3.230620000	2.167931000
H	-0.661419000	3.638922000	1.541337000
H	0.358720000	3.960216000	2.964439000
H	-0.217022000	2.310892000	2.651287000
C	2.378923000	4.579258000	0.611474000
H	3.312819000	4.465301000	0.039022000
H	2.602369000	5.198249000	1.494836000
H	1.663956000	5.134611000	-0.014452000
C	3.007632000	2.183958000	2.347466000
H	2.722613000	1.179205000	2.691917000
H	3.111082000	2.837889000	3.227588000
H	3.994260000	2.118252000	1.862824000
C	-0.815926000	3.621560000	-1.339938000
H	-1.500953000	3.090610000	-0.661248000
H	-1.376985000	3.917364000	-2.240072000
H	-0.492395000	4.537800000	-0.823544000
C	-0.022599000	1.213182000	-3.002728000
H	0.695059000	0.394266000	-3.164737000
H	-0.244651000	1.674137000	-3.977732000
H	-0.956765000	0.771121000	-2.627437000
C	1.903887000	3.529238000	-2.771133000
H	2.312714000	4.359554000	-2.178496000
H	1.434238000	3.949860000	-3.673992000
H	2.746773000	2.898590000	-3.094355000
C	3.321554000	-0.567831000	-2.590597000
H	2.774165000	-1.006551000	-3.440442000
H	4.389985000	-0.549274000	-2.857294000
H	2.986212000	0.472980000	-2.473353000
C	4.102396000	-0.881750000	0.366635000
H	4.027469000	-1.488811000	1.280355000
H	3.780192000	0.137246000	0.626198000
H	5.162327000	-0.836650000	0.071212000
C	3.799793000	-3.303699000	-1.468793000
H	3.752392000	-4.017605000	-0.633323000
H	4.857858000	-3.185362000	-1.750851000
H	3.271429000	-3.750632000	-2.325724000
C	2.069121000	-3.427009000	1.900855000
H	3.087052000	-3.609303000	1.527606000
H	1.768284000	-4.297381000	2.504806000
H	2.080746000	-2.544586000	2.559770000
C	0.660574000	-4.733866000	-0.514513000
H	-0.119876000	-4.622237000	-1.284450000
H	0.381322000	-5.586981000	0.123874000
H	1.601268000	-4.982411000	-1.025720000
C	-0.876866000	-2.971316000	1.412531000
H	-0.721710000	-2.833792000	2.493967000
H	-1.490626000	-3.875513000	1.273943000
H	-1.448683000	-2.106811000	1.047448000
C	-3.265334000	-1.250747000	-1.485926000
C	-2.022343000	-1.937226000	-2.064888000
H	-1.387199000	-1.252046000	-2.642876000
H	-2.357838000	-2.740015000	-2.738782000
H	-1.413577000	-2.384663000	-1.269015000
C	-4.055900000	-2.281483000	-0.670053000

H	-3.475125000	-2.666348000	0.179337000
H	-4.282087000	-3.131598000	-1.330966000
H	-5.012251000	-1.886466000	-0.303073000
C	-4.135278000	-0.691470000	-2.622645000
H	-5.017213000	-0.149740000	-2.251070000
H	-4.492776000	-1.532957000	-3.234480000
H	-3.561351000	-0.019198000	-3.277558000
C	-3.833652000	0.699158000	0.895527000
C	-3.866412000	-0.360251000	2.004911000
H	-4.452186000	-1.243612000	1.725797000
H	-4.333830000	0.084099000	2.896263000
H	-2.855315000	-0.687884000	2.286360000
C	-5.235171000	0.978959000	0.341055000
H	-5.215288000	1.724489000	-0.468871000
H	-5.853167000	1.390856000	1.152958000
H	-5.734635000	0.071852000	-0.025574000
C	-3.231349000	1.998608000	1.451954000
H	-2.205844000	1.844958000	1.812985000
H	-3.847529000	2.337960000	2.297647000
H	-3.219805000	2.802264000	0.699959000
H	-0.969948000	0.111527000	2.995803000
C	0.037935000	-0.366598000	3.091783000
O	0.760760000	-0.290634000	2.015094000
O	0.375222000	-0.889645000	4.122529000

7: E= -2146.2065376

Si	-3.140572000	-1.048225000	-0.160381000
Si	-2.037645000	1.921634000	0.253026000
Si	1.835476000	-0.782955000	1.745751000
Si	3.091268000	0.756929000	-0.751362000
Al	0.033810000	-0.260900000	-0.725889000
C	-1.840134000	0.249798000	-0.591416000
H	-2.051772000	0.461266000	-1.661834000
C	-2.608112000	-2.787818000	-0.668581000
H	-2.364828000	-2.825178000	-1.742154000
H	-3.432702000	-3.494259000	-0.485640000
H	-1.724162000	-3.140328000	-0.118329000
C	-4.722747000	-0.681766000	-1.127156000
H	-5.153960000	0.293970000	-0.862198000
H	-5.480642000	-1.454956000	-0.926212000
H	-4.522790000	-0.681105000	-2.210096000
C	-3.572667000	-1.082543000	1.676885000
H	-2.703244000	-1.339633000	2.299398000
H	-4.346424000	-1.847211000	1.847897000
H	-3.974454000	-0.118860000	2.024613000
C	-3.820035000	2.545853000	0.213825000
H	-4.199321000	2.600528000	-0.818122000
H	-3.869911000	3.557052000	0.646924000
H	-4.497871000	1.899699000	0.791943000
C	-1.486934000	1.884535000	2.060274000
H	-2.063334000	1.152828000	2.645433000
H	-1.646151000	2.876534000	2.511174000
H	-0.419610000	1.638352000	2.164641000
C	-0.983470000	3.187551000	-0.673910000
H	0.083360000	2.913130000	-0.681815000
H	-1.069155000	4.184377000	-0.214344000
H	-1.314697000	3.269921000	-1.721098000
C	1.567977000	0.379760000	0.283527000
H	1.267766000	1.347198000	0.730839000
C	0.165810000	-1.520030000	2.252492000
H	-0.554432000	-0.720334000	2.483456000

H	0.260931000	-2.157526000	3.144860000
H	-0.259606000	-2.147453000	1.450266000
C	2.522978000	0.153295000	3.230519000
H	3.498079000	0.609353000	3.006390000
H	2.650012000	-0.524252000	4.088935000
H	1.834313000	0.956934000	3.533981000
C	2.968775000	-2.225841000	1.308726000
H	2.526905000	-2.820797000	0.494381000
H	3.083706000	-2.883266000	2.184260000
H	3.972030000	-1.900268000	0.995212000
C	4.567310000	1.195921000	0.345054000
H	4.326396000	2.041969000	1.007359000
H	5.430835000	1.484494000	-0.274212000
H	4.874593000	0.348271000	0.976642000
C	2.741139000	2.233470000	-1.872310000
H	1.891530000	2.018151000	-2.539745000
H	3.614892000	2.462802000	-2.501831000
H	2.501583000	3.135176000	-1.287635000
C	3.583326000	-0.703457000	-1.857691000
H	3.327710000	-1.674049000	-1.407662000
H	4.668667000	-0.693651000	-2.039426000
H	3.081025000	-0.625719000	-2.832971000
O	0.405608000	-2.114349000	-1.194736000
O	0.449300000	-0.495230000	-2.620655000
C	0.600464000	-1.723207000	-2.378763000
H	0.894487000	-2.431318000	-3.170924000

7d: E= -4292.4446073

Si	-0.521562000	2.496914000	-3.911072000
Si	0.705010000	-0.249036000	-4.978819000
Si	4.163593000	1.389176000	-1.946216000
Si	3.522558000	-1.407737000	-0.608899000
Al	1.176310000	0.335054000	-1.929518000
O	1.028189000	1.641595000	-0.611295000
O	-0.214436000	1.032104000	1.128570000
C	0.097327000	0.761337000	-3.512406000
H	-0.842483000	0.238017000	-3.234840000
C	-0.629545000	3.618286000	-2.388960000
H	-1.256110000	3.171917000	-1.601256000
H	-1.083024000	4.580170000	-2.675443000
H	0.361512000	3.823877000	-1.959051000
C	-2.266532000	2.376530000	-4.638407000
H	-2.245279000	1.914257000	-5.636194000
H	-2.707903000	3.380245000	-4.742580000
H	-2.935456000	1.773532000	-4.006893000
C	0.504446000	3.408177000	-5.211780000
H	1.539699000	3.591973000	-4.893492000
H	0.033131000	4.384690000	-5.405992000
H	0.526924000	2.857396000	-6.164778000
C	-0.506213000	-0.212463000	-6.429328000
H	-1.516815000	-0.515175000	-6.114594000
H	-0.171589000	-0.906972000	-7.215726000
H	-0.576079000	0.790984000	-6.876219000
C	2.379814000	0.323058000	-5.641070000
H	2.342762000	1.373687000	-5.964939000
H	2.655961000	-0.288541000	-6.514191000
H	3.183055000	0.225645000	-4.896265000
C	0.856844000	-2.056325000	-4.429604000
H	1.594023000	-2.187705000	-3.621289000
H	1.164737000	-2.697991000	-5.269372000
H	-0.113953000	-2.425605000	-4.061599000

C	3.078046000	-0.148484000	-1.923937000
H	3.267957000	-0.649257000	-2.892549000
C	3.320934000	2.764395000	-2.928889000
H	3.083405000	2.414708000	-3.944172000
H	3.971662000	3.648156000	-3.015258000
H	2.382178000	3.084762000	-2.449115000
C	5.814895000	1.040143000	-2.792923000
H	6.396762000	0.271723000	-2.264413000
H	6.421937000	1.957701000	-2.838296000
H	5.652410000	0.693086000	-3.825378000
C	4.492261000	2.066132000	-0.211704000
H	3.549796000	2.336185000	0.288175000
H	5.105188000	2.977931000	-0.285411000
H	5.030001000	1.353420000	0.430982000
C	5.384800000	-1.634605000	-0.374484000
H	5.856770000	-1.965567000	-1.312627000
H	5.568987000	-2.409540000	0.386027000
H	5.889584000	-0.714286000	-0.046186000
C	2.863456000	-3.117157000	-1.077373000
H	1.777480000	-3.118554000	-1.244518000
H	3.091214000	-3.853305000	-0.290692000
H	3.342360000	-3.462474000	-2.007536000
C	2.789251000	-0.893263000	1.056687000
H	3.125191000	0.113411000	1.349255000
H	3.097786000	-1.597037000	1.843943000
H	1.688684000	-0.890541000	1.029051000
C	0.500382000	1.839085000	0.506268000
H	0.688851000	2.824487000	0.971574000
Si	0.521562000	-2.496914000	3.911072000
Si	-0.705010000	0.249036000	4.978819000
Si	-4.163593000	-1.389176000	1.946216000
Si	-3.522558000	1.407737000	0.608899000
Al	-1.176310000	-0.335054000	1.929518000
O	-1.028189000	-1.641595000	0.611295000
O	0.214436000	-1.032104000	-1.128570000
C	-0.097327000	-0.761337000	3.512406000
H	0.842483000	-0.238017000	3.234840000
C	0.629545000	-3.618286000	2.388960000
H	1.256110000	-3.171917000	1.601256000
H	1.083024000	-4.580170000	2.675443000
H	-0.361512000	-3.823877000	1.959051000
C	2.266532000	-2.376530000	4.638407000
H	2.245279000	-1.914257000	5.636194000
H	2.707903000	-3.380245000	4.742580000
H	2.935456000	-1.773532000	4.006893000
C	-0.504446000	-3.408177000	5.211780000
H	-1.539699000	-3.591973000	4.893492000
H	-0.033131000	-4.384690000	5.405992000
H	-0.526924000	-2.857396000	6.164778000
C	0.506213000	0.212463000	6.429328000
H	1.516815000	0.515175000	6.114594000
H	0.171589000	0.906972000	7.215726000
H	0.576079000	-0.790984000	6.876219000
C	-2.379814000	-0.323058000	5.641070000
H	-2.342762000	-1.373687000	5.964939000
H	-2.655961000	0.288541000	6.514191000
H	-3.183055000	-0.225645000	4.896265000
C	-0.856844000	2.056325000	4.429604000
H	-1.594023000	2.187705000	3.621289000
H	-1.164737000	2.697991000	5.269372000
H	0.113953000	2.425605000	4.061599000

C	-3.078046000	0.148484000	1.923937000
H	-3.267957000	0.649257000	2.892549000
C	-3.320934000	-2.764395000	2.928889000
H	-3.083405000	-2.414708000	3.944172000
H	-3.971662000	-3.648156000	3.015258000
H	-2.382178000	-3.084762000	2.449115000
C	-5.814895000	-1.040143000	2.792923000
H	-6.396762000	-0.271723000	2.264413000
H	-6.421937000	-1.957701000	2.838296000
H	-5.652410000	-0.693086000	3.825378000
C	-4.492261000	-2.066132000	0.211704000
H	-3.549796000	-2.336185000	-0.288175000
H	-5.105188000	-2.977931000	0.285411000
H	-5.030001000	-1.353420000	-0.430982000
C	-5.384800000	1.634605000	0.374484000
H	-5.856770000	1.965567000	1.312627000
H	-5.568987000	2.409540000	-0.386027000
H	-5.889584000	0.714286000	0.046186000
C	-2.863456000	3.117157000	1.077373000
H	-1.777480000	3.118554000	1.244518000
H	-3.091214000	3.853305000	0.290692000
H	-3.342360000	3.462474000	2.007536000
C	-2.789251000	0.893263000	-1.056687000
H	-3.125191000	-0.113411000	-1.349255000
H	-3.097786000	1.597037000	-1.843943000
H	-1.688684000	0.890541000	-1.029051000
C	-0.500382000	-1.839085000	-0.506268000
H	-0.688851000	-2.824487000	-0.971574000

8: E= -2879.0774635

P	-2.629500000	-0.814626000	0.222847000
H	-1.158491000	-0.699011000	1.856888000
Si	1.518699000	2.793944000	1.297232000
Si	0.300802000	2.814167000	-1.640371000
Si	3.041098000	-1.278740000	-1.326423000
Si	1.472431000	-3.068257000	0.738809000
Al	0.362205000	0.012225000	-0.019048000
O	-1.336618000	-0.113708000	-0.493647000
C	1.111589000	1.817181000	-0.248521000
H	2.119888000	1.600366000	-0.654513000
C	1.395602000	-1.613682000	-0.463186000
H	0.751515000	-1.991598000	-1.287445000
C	0.015736000	3.158840000	2.388045000
H	-0.690880000	3.808331000	1.849057000
H	0.344792000	3.698956000	3.289679000
H	-0.550355000	2.274420000	2.710390000
C	2.303297000	4.473987000	0.931999000
H	3.206463000	4.359954000	0.312815000
H	2.601246000	4.955596000	1.876676000
H	1.615569000	5.155681000	0.409795000
C	2.835403000	1.849380000	2.300814000
H	2.793903000	0.756455000	2.167122000
H	2.772056000	2.077199000	3.376927000
H	3.836758000	2.158528000	1.962461000
C	-1.024796000	4.012647000	-1.021956000
H	-1.844999000	3.500532000	-0.498253000
H	-1.459265000	4.534396000	-1.889295000
H	-0.612992000	4.778373000	-0.347247000
C	-0.499309000	1.720966000	-2.956062000
H	0.225592000	1.019113000	-3.395839000
H	-0.893513000	2.349391000	-3.770015000

H	-1.320306000	1.129982000	-2.527696000
C	1.625603000	3.836407000	-2.523346000
H	2.110166000	4.556966000	-1.849429000
H	1.175251000	4.397708000	-3.357075000
H	2.408943000	3.186270000	-2.943502000
C	2.756217000	-0.278679000	-2.906375000
H	2.045024000	-0.793767000	-3.571555000
H	3.704860000	-0.164331000	-3.453663000
H	2.362906000	0.728542000	-2.707192000
C	4.278354000	-0.334497000	-0.252256000
H	4.467723000	-0.838932000	0.706438000
H	3.952082000	0.692078000	-0.033835000
H	5.236587000	-0.269714000	-0.791719000
C	3.924897000	-2.852541000	-1.897661000
H	4.236972000	-3.498454000	-1.063783000
H	4.830140000	-2.565617000	-2.455665000
H	3.290372000	-3.447691000	-2.572089000
C	3.012668000	-2.969132000	1.831221000
H	3.947461000	-3.048814000	1.257498000
H	2.995517000	-3.789221000	2.565578000
H	3.040838000	-2.020376000	2.391440000
C	1.481089000	-4.700970000	-0.216467000
H	0.531709000	-4.821394000	-0.762577000
H	1.567864000	-5.543968000	0.486753000
H	2.300506000	-4.774836000	-0.942626000
C	0.016007000	-3.251438000	1.946257000
H	0.149943000	-2.683250000	2.878183000
H	-0.040008000	-4.313756000	2.232939000
H	-0.958444000	-2.980014000	1.513412000
C	-3.796515000	0.650827000	0.399024000
C	-3.015533000	1.606657000	1.313942000
H	-2.826002000	1.153334000	2.301709000
H	-3.596398000	2.529194000	1.476014000
H	-2.051405000	1.885557000	0.864771000
C	-4.114461000	1.364557000	-0.914050000
H	-3.191852000	1.599891000	-1.466600000
H	-4.636535000	2.313306000	-0.705444000
H	-4.768963000	0.762847000	-1.561271000
C	-5.075673000	0.228285000	1.130150000
H	-5.750295000	-0.360673000	0.496333000
H	-5.624213000	1.128276000	1.451937000
H	-4.844176000	-0.362012000	2.030988000
C	-3.207065000	-1.974434000	-1.144454000
C	-2.905558000	-1.414375000	-2.536311000
H	-3.425021000	-0.467154000	-2.731252000
H	-3.230939000	-2.143675000	-3.296374000
H	-1.828358000	-1.238997000	-2.661407000
C	-4.693182000	-2.307874000	-1.001449000
H	-4.952169000	-2.601915000	0.028108000
H	-4.940859000	-3.154577000	-1.661707000
H	-5.331001000	-1.461942000	-1.294007000
C	-2.385362000	-3.257462000	-0.947357000
H	-1.304717000	-3.041205000	-0.947595000
H	-2.588603000	-3.960577000	-1.771258000
H	-2.633975000	-3.757372000	0.000936000
H	1.124819000	0.331565000	3.311332000
C	0.113385000	-0.101692000	3.230307000
O	-0.250454000	-0.256129000	1.925982000
O	-0.604886000	-0.405268000	4.123581000

TS(AI): E= -2690.4261940

P	-0.303177000	2.512522000	-0.426766000
Si	-1.950291000	-2.124563000	1.633828000
Al	0.021924000	-0.408947000	-0.243878000
O	-0.107269000	1.235730000	0.521544000
C	-1.798874000	3.401648000	0.234753000
C	-2.894224000	2.328826000	0.264894000
H	-2.608770000	1.479624000	0.901109000
H	-3.823399000	2.766987000	0.662864000
H	-3.108604000	1.949563000	-0.745878000
C	-2.226814000	4.521528000	-0.720178000
H	-1.520623000	5.361098000	-0.733207000
H	-2.345106000	4.148026000	-1.748900000
H	-3.202422000	4.912668000	-0.391386000
C	-1.561182000	3.934876000	1.649404000
H	-0.852686000	4.775203000	1.657552000
H	-2.515116000	4.300423000	2.062507000
H	-1.181956000	3.144173000	2.313729000
C	1.287607000	3.472890000	-0.284717000
C	2.247764000	2.701264000	-1.202344000
H	1.941872000	2.765750000	-2.257531000
H	3.263994000	3.117535000	-1.112037000
H	2.296453000	1.636277000	-0.924716000
C	1.833748000	3.448819000	1.144857000
H	1.940457000	2.417829000	1.507386000
H	2.828590000	3.923275000	1.153784000
H	1.191932000	3.996945000	1.847191000
C	1.136411000	4.908002000	-0.792961000
H	0.661883000	4.947745000	-1.785973000
H	0.554628000	5.531753000	-0.099616000
H	2.136867000	5.358990000	-0.884850000
C	1.745787000	-1.343968000	-0.004013000
C	3.954997000	-3.015500000	-1.456842000
H	3.659868000	-3.902832000	-0.875565000
H	4.306640000	-3.355610000	-2.443440000
H	4.805446000	-2.542376000	-0.941866000
C	3.120277000	-0.348358000	-2.670206000
H	3.599566000	-0.721039000	-3.589183000
H	2.288821000	0.308515000	-2.965972000
H	3.859847000	0.255503000	-2.123666000
C	2.083712000	0.060247000	2.816432000
H	2.796486000	0.750222000	3.295678000
H	1.200610000	0.640036000	2.508470000
C	3.717090000	-2.382778000	2.120300000
H	4.357004000	-2.110223000	2.974399000
H	2.935898000	-3.065967000	2.490128000
H	4.332191000	-2.931723000	1.392833000
H	0.038894000	-3.619789000	1.968571000
H	-4.168937000	-3.292964000	1.246189000
C	-2.595533000	-0.664606000	2.642557000
H	-2.785654000	-0.972809000	3.682310000
H	-1.848499000	0.145545000	2.658729000
H	-3.533268000	-0.261621000	2.232295000
C	-3.453914000	-3.095425000	-1.994087000
H	-4.327881000	-3.031592000	-2.660634000
H	-3.680520000	-3.822339000	-1.199715000
C	-2.681640000	-0.274321000	-2.746844000
H	-3.574589000	-0.237208000	-3.390818000
H	-2.430724000	0.757827000	-2.457973000
H	-1.844772000	-0.659350000	-3.349591000
Si	2.503513000	-1.817907000	-1.654439000
Si	2.928699000	-0.836224000	1.365965000

Si	-3.018861000	-1.405125000	-1.266943000
H	1.363114000	-2.322336000	0.355225000
C	1.182898000	-2.700824000	-2.686695000
H	1.594773000	-3.036974000	-3.650762000
H	0.796294000	-3.586361000	-2.157166000
H	0.330149000	-2.035151000	-2.900910000
H	1.767493000	-0.662510000	3.583664000
C	4.349530000	0.257717000	0.757208000
H	4.011638000	1.228801000	0.368562000
H	5.032835000	0.453446000	1.598428000
H	4.929188000	-0.243438000	-0.033469000
C	-1.536174000	-1.620062000	-0.127086000
C	-0.407638000	-2.773260000	2.514219000
H	0.358559000	-1.991250000	2.617473000
H	-0.669385000	-3.122709000	3.525230000
C	-3.203127000	-3.541739000	1.708509000
H	-3.392608000	-3.819714000	2.757193000
H	-2.802488000	-4.429385000	1.193839000
C	-4.576319000	-0.755601000	-0.406119000
H	-5.380008000	-0.660039000	-1.153361000
H	-4.929742000	-1.445678000	0.374013000
H	-4.432921000	0.229098000	0.058789000
H	-2.608138000	-3.488486000	-2.580425000
H	-1.048663000	-2.530551000	-0.538467000
H	-0.257518000	1.408620000	-1.701682000
H	-0.015327000	0.390424000	-1.853816000

TS(Ga): E= -4372.8237199

P	-0.874357000	2.402644000	-0.386378000
Si	-1.373577000	-2.566349000	1.556989000
Ga	0.151750000	-0.443704000	-0.304094000
O	-0.357721000	1.209710000	0.542019000
C	-2.535556000	2.892817000	0.310697000
C	-3.309265000	1.574500000	0.422948000
H	-2.789599000	0.865811000	1.082413000
H	-4.311995000	1.770680000	0.835104000
H	-3.440487000	1.101761000	-0.561646000
C	-3.270353000	3.823893000	-0.659564000
H	-2.789839000	4.806512000	-0.751995000
H	-3.344484000	3.377712000	-1.663186000
H	-4.294641000	3.987857000	-0.288866000
C	-2.408893000	3.524348000	1.699221000
H	-1.941268000	4.518349000	1.659307000
H	-3.413891000	3.646963000	2.134403000
H	-1.821365000	2.882864000	2.372895000
C	0.414030000	3.746856000	-0.225773000
C	1.535185000	3.291122000	-1.171738000
H	1.210693000	3.303689000	-2.223447000
H	2.403821000	3.961845000	-1.071540000
H	1.871745000	2.270940000	-0.931557000
C	0.968498000	3.824768000	1.198865000
H	1.328015000	2.841475000	1.530934000
H	1.818784000	4.526202000	1.214752000
H	0.223473000	4.182369000	1.921604000
C	-0.116093000	5.105526000	-0.687879000
H	-0.582127000	5.048227000	-1.684063000
H	-0.846911000	5.524415000	0.018008000
H	0.725381000	5.813133000	-0.754011000
C	2.067988000	-0.965237000	-0.026487000
C	4.684938000	-1.919252000	-1.434643000
H	4.607258000	-2.878030000	-0.899016000

H	5.147737000	-2.111467000	-2.415237000
H	5.364538000	-1.266939000	-0.864696000
C	3.228599000	0.511795000	-2.565591000
H	3.806557000	0.331701000	-3.485700000
H	2.264581000	0.955206000	-2.856140000
H	3.778374000	1.246931000	-1.959462000
C	1.812426000	0.298435000	2.831935000
H	2.371977000	0.821554000	3.623519000
H	1.011199000	0.958273000	2.468193000
C	4.144931000	-1.518395000	2.170668000
H	4.668204000	-1.116690000	3.052476000
H	3.578532000	-2.407000000	2.491208000
H	4.901714000	-1.844939000	1.442925000
H	0.647252000	-4.050119000	1.494049000
H	-3.639287000	-3.667048000	1.387081000
C	-1.884278000	-1.175170000	2.730114000
H	-1.766665000	-1.500456000	3.775500000
H	-1.262511000	-0.278230000	2.575833000
H	-2.937107000	-0.887841000	2.588769000
C	-2.965666000	-3.611237000	-2.049944000
H	-3.866772000	-3.630727000	-2.682602000
H	-3.074700000	-4.390220000	-1.280189000
C	-2.628989000	-0.684897000	-2.703676000
H	-3.547821000	-0.754090000	-3.307466000
H	-2.513464000	0.362139000	-2.383332000
H	-1.775430000	-0.925254000	-3.356740000
Si	2.983665000	-1.125660000	-1.658127000
Si	2.983353000	-0.217467000	1.437906000
Si	-2.735988000	-1.908003000	-1.261187000
H	1.939102000	-2.026395000	0.268266000
C	1.960771000	-2.252271000	-2.785042000
H	2.448132000	-2.394101000	-3.761763000
H	1.822390000	-3.244691000	-2.327272000
H	0.961346000	-1.823341000	-2.969167000
H	1.333634000	-0.580558000	3.291384000
C	4.045623000	1.273085000	0.960834000
H	3.463153000	2.094985000	0.520845000
H	4.549353000	1.662182000	1.859519000
H	4.826230000	0.985069000	0.239445000
C	-1.172138000	-1.951537000	-0.211930000
C	0.265060000	-3.278973000	2.181641000
H	1.042019000	-2.508869000	2.290289000
H	0.118479000	-3.747945000	3.167211000
C	-2.629952000	-3.972350000	1.698076000
H	-2.687836000	-4.314804000	2.743303000
H	-2.325625000	-4.831513000	1.080456000
C	-4.322674000	-1.534084000	-0.280654000
H	-4.987145000	-0.877982000	-0.863773000
H	-4.873391000	-2.465377000	-0.080582000
H	-4.131393000	-1.043778000	0.684102000
H	-2.101465000	-3.872869000	-2.680326000
H	-0.574467000	-2.753248000	-0.694446000
H	-0.545636000	1.348699000	-1.708793000
H	-0.082974000	0.456693000	-1.890961000

TS(In): E= -2638.0204649

P	-0.332371000	2.698484000	-0.349986000
Si	-2.038948000	-2.376650000	1.519881000
In	0.019822000	-0.507840000	-0.342054000
O	-0.150906000	1.426577000	0.587675000
C	-1.815564000	3.614585000	0.328358000

C	-2.908023000	2.544737000	0.441332000
H	-2.606424000	1.740372000	1.127573000
H	-3.834807000	3.004364000	0.820692000
H	-3.133797000	2.099074000	-0.539911000
C	-2.274531000	4.694475000	-0.657163000
H	-1.556518000	5.520197000	-0.743991000
H	-2.440701000	4.273292000	-1.660515000
H	-3.229077000	5.118527000	-0.306689000
C	-1.545242000	4.206627000	1.713242000
H	-0.830488000	5.040788000	1.672568000
H	-2.487623000	4.596537000	2.131851000
H	-1.156911000	3.441131000	2.401227000
C	1.259886000	3.669909000	-0.184846000
C	2.232759000	2.929864000	-1.114598000
H	1.922932000	3.001493000	-2.168377000
H	3.242570000	3.361962000	-1.021829000
H	2.303758000	1.862753000	-0.852673000
C	1.804408000	3.619502000	1.244647000
H	1.892843000	2.581127000	1.592585000
H	2.807171000	4.077442000	1.265638000
H	1.168477000	4.166281000	1.952933000
C	1.106216000	5.113787000	-0.665983000
H	0.650117000	5.167008000	-1.667126000
H	0.503243000	5.718828000	0.025946000
H	2.103124000	5.578286000	-0.730205000
C	1.983768000	-1.445198000	-0.002315000
C	4.446634000	-2.772812000	-1.367684000
H	4.208483000	-3.723398000	-0.865886000
H	4.916740000	-3.007182000	-2.335396000
H	5.190578000	-2.243544000	-0.752445000
C	3.383987000	-0.131571000	-2.492175000
H	3.926474000	-0.371915000	-3.419840000
H	2.493902000	0.455928000	-2.764796000
H	4.035923000	0.500476000	-1.871386000
C	1.825215000	-0.083797000	2.807664000
H	2.423195000	0.369038000	3.614268000
H	1.172273000	0.691823000	2.377296000
C	3.832609000	-2.312719000	2.288822000
H	4.383550000	-1.998457000	3.189115000
H	3.102681000	-3.080121000	2.591119000
H	4.547988000	-2.780543000	1.596123000
H	-0.228103000	-4.106700000	1.487464000
H	-4.417002000	-3.218459000	1.316746000
C	-2.378501000	-0.901979000	2.647829000
H	-2.436953000	-1.218740000	3.700573000
H	-1.576450000	-0.149611000	2.562514000
H	-3.328760000	-0.411829000	2.388213000
C	-4.026018000	-2.861890000	-2.019405000
H	-4.926878000	-2.614233000	-2.602181000
H	-4.305525000	-3.606443000	-1.258731000
C	-2.902119000	-0.106010000	-2.625598000
H	-3.812209000	0.105245000	-3.208740000
H	-2.507744000	0.854110000	-2.256293000
H	-2.151174000	-0.528284000	-3.312212000
Si	2.891444000	-1.729205000	-1.617431000
Si	2.953208000	-0.840049000	1.491679000
Si	-3.293762000	-1.311837000	-1.222143000
H	1.648985000	-2.462759000	0.284103000
C	1.731743000	-2.672417000	-2.780172000
H	2.236323000	-2.934695000	-3.722752000
H	1.379903000	-3.606220000	-2.313632000

H	0.844904000	-2.068576000	-3.039279000
H	1.181355000	-0.850188000	3.267046000
C	4.272146000	0.434641000	1.036127000
H	3.843035000	1.340795000	0.584997000
H	4.814712000	0.738558000	1.945019000
H	5.008427000	0.017487000	0.331446000
C	-1.762442000	-1.803786000	-0.247860000
C	-0.497742000	-3.272429000	2.154599000
H	0.373498000	-2.604436000	2.225788000
H	-0.681563000	-3.688482000	3.157410000
C	-3.452974000	-3.625547000	1.654065000
H	-3.571564000	-3.953821000	2.698395000
H	-3.230641000	-4.515991000	1.045079000
C	-4.653382000	-0.539450000	-0.157565000
H	-5.492344000	-0.244203000	-0.807339000
H	-5.043565000	-1.252948000	0.583095000
H	-4.316630000	0.355335000	0.382568000
H	-3.299698000	-3.330183000	-2.701829000
H	-1.370614000	-2.695331000	-0.779485000
H	-0.254502000	1.617413000	-1.732748000
H	-0.021535000	0.683136000	-1.989800000

TS4-5: E= -2877.8918592

P	-1.766479000	-1.871792000	0.237326000
Si	-0.363147000	2.944785000	-1.648332000
Al	0.340216000	0.352280000	0.060109000
O	-0.671906000	-0.951509000	-0.552953000
O	0.043663000	-0.276788000	2.020508000
O	-1.201102000	-1.528701000	3.512823000
C	-0.676160000	-0.958333000	2.664381000
C	-3.275123000	-1.628180000	-0.860520000
C	-3.714704000	-0.196508000	-0.524450000
H	-2.894022000	0.512204000	-0.717634000
H	-4.568886000	0.095766000	-1.157323000
H	-4.019714000	-0.100667000	0.529192000
C	-4.385809000	-2.609239000	-0.484181000
H	-4.141661000	-3.638736000	-0.784418000
H	-4.586963000	-2.600125000	0.598938000
H	-5.316791000	-2.325961000	-1.001177000
C	-2.950373000	-1.700313000	-2.356213000
H	-2.876300000	-2.732871000	-2.717106000
H	-3.752823000	-1.206118000	-2.927963000
H	-2.004180000	-1.185292000	-2.577439000
C	-1.084139000	-3.615941000	0.049898000
C	0.377789000	-3.515881000	0.505003000
H	0.467241000	-3.122947000	1.531732000
H	0.836423000	-4.517873000	0.500668000
H	0.958564000	-2.865781000	-0.164004000
C	-1.127194000	-4.201123000	-1.361649000
H	-0.691665000	-3.513138000	-2.100351000
H	-0.548822000	-5.139462000	-1.388130000
H	-2.154614000	-4.438565000	-1.671077000
C	-1.843601000	-4.519186000	1.030215000
H	-1.785148000	-4.128212000	2.057598000
H	-2.905325000	-4.623290000	0.765663000
H	-1.397663000	-5.526869000	1.022618000
C	2.283099000	0.206640000	-0.156520000
C	5.092332000	0.507368000	1.147019000
H	5.243291000	1.444475000	0.588662000
H	5.625923000	0.597329000	2.106222000
H	5.565111000	-0.305746000	0.575992000

C	3.094512000	-1.408338000	2.432925000
H	2.100592000	-1.525272000	2.887346000
H	3.286680000	-2.287994000	1.801919000
H	3.832816000	-1.412202000	3.250033000
C	1.656606000	-1.404389000	-2.781033000
H	2.113104000	-1.996634000	-3.589405000
H	0.875611000	-2.006354000	-2.295870000
C	4.291362000	0.102246000	-2.475913000
H	4.705944000	-0.495357000	-3.302551000
H	3.863059000	1.021902000	-2.903125000
H	5.121069000	0.391612000	-1.813881000
H	2.122636000	3.035285000	-2.009029000
H	-1.471101000	5.182883000	-1.160566000
C	-1.740639000	2.182316000	-2.686507000
H	-1.725245000	2.597029000	-3.706174000
H	-1.600875000	1.092061000	-2.760765000
H	-2.736054000	2.365512000	-2.257104000
C	-1.078109000	4.411433000	2.047148000
H	-1.840278000	4.832465000	2.720747000
H	-0.807038000	5.183956000	1.311834000
C	-2.227513000	1.660456000	2.579556000
H	-3.075111000	2.101006000	3.127369000
H	-2.561704000	0.686281000	2.186864000
H	-1.415557000	1.502146000	3.306289000
Si	3.249979000	0.202834000	1.453655000
Si	2.977628000	-0.878401000	-1.533975000
Si	-1.707828000	2.846127000	1.195647000
H	2.491066000	1.231132000	-0.529039000
C	2.660772000	1.634393000	2.546830000
H	3.235377000	1.664722000	3.485603000
H	2.812089000	2.597072000	2.032510000
H	1.593926000	1.555024000	2.807305000
H	1.154915000	-0.538901000	-3.241680000
C	3.813297000	-2.460054000	-0.914385000
H	3.117367000	-3.140814000	-0.403784000
H	4.234130000	-2.998623000	-1.777929000
H	4.640724000	-2.239587000	-0.223588000
C	-0.322123000	2.206474000	0.085614000
C	1.263287000	2.622384000	-2.561163000
H	1.451009000	1.551015000	-2.725457000
H	1.233185000	3.110049000	-3.548109000
C	-0.537593000	4.829068000	-1.620717000
H	-0.502448000	5.218330000	-2.650296000
H	0.301951000	5.277528000	-1.066087000
C	-3.317589000	3.294936000	0.303772000
H	-3.995004000	3.750997000	1.043020000
H	-3.173732000	4.022835000	-0.506696000
H	-3.828416000	2.416729000	-0.114654000
H	-0.181455000	4.187216000	2.646633000
H	0.576730000	2.685887000	0.530725000

TS1-7: E= -2146.1243710

Si	3.117878000	1.015698000	0.224413000
Si	2.083348000	-1.911342000	-0.541992000
Si	-1.765038000	-0.084092000	1.891650000
Si	-3.099608000	-0.531014000	-0.971243000
Al	-0.056237000	0.398331000	-0.718767000
C	1.847801000	-0.045912000	-0.682889000
H	2.096080000	0.158907000	-1.746369000
C	2.556853000	2.809552000	0.432758000
H	2.294778000	3.259460000	-0.538848000

H	3.385946000	3.399489000	0.853826000
H	1.693564000	2.915188000	1.105134000
C	4.696422000	1.086559000	-0.813203000
H	5.142227000	0.091022000	-0.950308000
H	5.445456000	1.730452000	-0.326628000
H	4.489107000	1.506382000	-1.810030000
C	3.582438000	0.348602000	1.927872000
H	2.723388000	0.314889000	2.612903000
H	4.342896000	1.009792000	2.372071000
H	4.015771000	-0.661141000	1.864862000
C	3.875200000	-2.430310000	-0.833156000
H	4.239644000	-2.065108000	-1.805612000
H	3.949228000	-3.528962000	-0.833630000
H	4.549564000	-2.048932000	-0.051723000
C	1.553392000	-2.591077000	1.138333000
H	2.130063000	-2.139620000	1.959048000
H	1.727490000	-3.678053000	1.162945000
H	0.485176000	-2.418733000	1.338080000
C	1.039195000	-2.743266000	-1.882755000
H	1.353737000	-2.404593000	-2.882585000
H	-0.035040000	-2.521508000	-1.776955000
H	1.154524000	-3.837546000	-1.847336000
C	-1.544817000	-0.576886000	0.084198000
H	-1.229584000	-1.638143000	0.111079000
C	-0.099380000	0.418609000	2.635284000
H	0.624866000	-0.405142000	2.553196000
H	-0.206181000	0.670201000	3.701707000
H	0.327597000	1.301019000	2.130832000
C	-2.413605000	-1.544122000	2.893455000
H	-3.391591000	-1.885269000	2.524496000
H	-2.524063000	-1.268557000	3.953599000
H	-1.714613000	-2.393062000	2.836847000
C	-2.930707000	1.385910000	2.100027000
H	-2.529852000	2.278461000	1.596580000
H	-3.030746000	1.621194000	3.170919000
H	-3.937844000	1.189533000	1.703258000
C	-4.572922000	-1.332575000	-0.099518000
H	-4.344245000	-2.374992000	0.172229000
H	-5.448078000	-1.342597000	-0.767686000
H	-4.859293000	-0.798399000	0.819184000
C	-2.800291000	-1.486767000	-2.571203000
H	-1.961484000	-1.057046000	-3.141455000
H	-3.693068000	-1.459220000	-3.214919000
H	-2.567657000	-2.543012000	-2.363838000
C	-3.567592000	1.244581000	-1.431743000
H	-3.511579000	1.926873000	-0.570163000
H	-4.600593000	1.274209000	-1.811325000
H	-2.917955000	1.632573000	-2.230930000
O	-0.471073000	2.314058000	-0.108167000
O	-0.863154000	3.562563000	-2.019675000
C	-0.649110000	2.783930000	-1.199451000
H	-0.412105000	1.188244000	-2.133388000

TS3-6: E= -2879.0525710

P	-2.782795000	0.528571000	-0.471467000
H	-2.877268000	1.629254000	-1.355658000
Si	2.135192000	2.686211000	1.054651000
Si	0.925894000	2.428230000	-1.872464000
Si	2.771497000	-2.024449000	-1.066294000
Si	0.349241000	-3.264810000	0.528763000
Al	0.492044000	-0.030557000	0.137933000

O	-1.298965000	0.164402000	-0.282308000
C	1.577040000	1.553113000	-0.346050000
H	2.519018000	1.075511000	-0.680487000
C	0.987192000	-1.826443000	-0.510190000
H	0.387846000	-1.882837000	-1.444191000
C	0.717441000	3.196858000	2.195039000
H	-0.053045000	3.757626000	1.643469000
H	1.109649000	3.860169000	2.981755000
H	0.241901000	2.337694000	2.692672000
C	2.916200000	4.299421000	0.433300000
H	3.808121000	4.096328000	-0.179373000
H	3.236979000	4.895736000	1.302299000
H	2.228248000	4.919260000	-0.160882000
C	3.481371000	1.852590000	2.076988000
H	3.161872000	0.886264000	2.491695000
H	3.777001000	2.507863000	2.911360000
H	4.374775000	1.679481000	1.455862000
C	-0.377258000	3.714493000	-1.394485000
H	-1.147826000	3.265091000	-0.749456000
H	-0.872477000	4.126275000	-2.287527000
H	0.064933000	4.554080000	-0.837092000
C	0.099389000	1.221738000	-3.079661000
H	0.779279000	0.396255000	-3.340852000
H	-0.180636000	1.740101000	-4.009816000
H	-0.807036000	0.781542000	-2.642991000
C	2.293432000	3.270658000	-2.865308000
H	2.811399000	4.047575000	-2.287714000
H	1.870104000	3.737263000	-3.768557000
H	3.042373000	2.531902000	-3.191328000
C	3.144225000	-0.983519000	-2.607844000
H	2.494669000	-1.290768000	-3.443190000
H	4.186303000	-1.159327000	-2.918696000
H	3.018562000	0.098466000	-2.460333000
C	3.958037000	-1.541598000	0.313418000
H	3.787251000	-2.154261000	1.210383000
H	3.814600000	-0.492526000	0.613310000
H	5.004134000	-1.669145000	-0.004849000
C	3.168262000	-3.790115000	-1.633082000
H	3.018025000	-4.548536000	-0.851824000
H	4.220955000	-3.842373000	-1.953346000
H	2.543917000	-4.065462000	-2.497942000
C	1.606204000	-3.985163000	1.734144000
H	2.499736000	-4.394009000	1.241950000
H	1.126869000	-4.803082000	2.295270000
H	1.921798000	-3.213637000	2.450586000
C	-0.243263000	-4.641943000	-0.631536000
H	-1.073976000	-4.291512000	-1.265165000
H	-0.604126000	-5.506970000	-0.053205000
H	0.562183000	-4.987544000	-1.295884000
C	-1.171301000	-2.773663000	1.555800000
H	-0.911761000	-2.338474000	2.532256000
H	-1.806698000	-3.654026000	1.742523000
H	-1.768095000	-2.025789000	1.015164000
C	-3.705220000	-0.810455000	-1.359768000
C	-2.690397000	-1.495771000	-2.285989000
H	-2.248794000	-0.794683000	-3.009414000
H	-3.212848000	-2.282039000	-2.851319000
H	-1.875714000	-1.959547000	-1.711924000
C	-4.319161000	-1.854302000	-0.418240000
H	-3.560810000	-2.361954000	0.191770000
H	-4.812233000	-2.618981000	-1.036914000

H	-5.079434000	-1.425018000	0.247469000
C	-4.809864000	-0.145263000	-2.195669000
H	-5.555729000	0.368582000	-1.573491000
H	-5.334362000	-0.928996000	-2.762280000
H	-4.400267000	0.573919000	-2.919853000
C	-3.513720000	1.137901000	1.100817000
C	-3.287589000	0.115465000	2.221390000
H	-3.776510000	-0.847481000	2.023626000
H	-3.714495000	0.526402000	3.148772000
H	-2.216449000	-0.056111000	2.404920000
C	-4.999783000	1.459351000	0.908551000
H	-5.165929000	2.166341000	0.081002000
H	-5.368442000	1.937955000	1.828107000
H	-5.608628000	0.561345000	0.736732000
C	-2.743997000	2.423295000	1.433202000
H	-1.664750000	2.234008000	1.511265000
H	-3.085987000	2.794240000	2.410930000
H	-2.919441000	3.214135000	0.688107000
H	0.199424000	0.016190000	1.803604000
C	0.676788000	-0.405370000	3.072873000
O	1.744700000	-0.923156000	2.924688000
O	-0.182298000	-0.085409000	3.837141000

TS6-8: E= -2879.0739216

P	-2.592875000	-0.672935000	0.053110000
H	-1.549836000	-0.709339000	1.457597000
Si	1.541126000	2.659344000	1.421989000
Si	0.480860000	2.881833000	-1.578866000
Si	3.034839000	-1.319267000	-1.286970000
Si	1.453219000	-3.083395000	0.776234000
Al	0.348393000	-0.001059000	-0.001930000
O	-1.303625000	-0.094476000	-0.725774000
C	1.149029000	1.788479000	-0.189078000
H	2.162663000	1.529176000	-0.554399000
C	1.383475000	-1.635660000	-0.432333000
H	0.748996000	-2.018733000	-1.261179000
C	0.012368000	3.143033000	2.426590000
H	-0.622109000	3.832243000	1.848766000
H	0.336335000	3.670039000	3.337902000
H	-0.622300000	2.301560000	2.734943000
C	2.518436000	4.259236000	1.178169000
H	3.432123000	4.079917000	0.590475000
H	2.821383000	4.662626000	2.157367000
H	1.928710000	5.033546000	0.664424000
C	2.665481000	1.527717000	2.464487000
H	2.491549000	0.454005000	2.280960000
H	2.552094000	1.719925000	3.543162000
H	3.719065000	1.718494000	2.207217000
C	-0.772872000	4.168837000	-0.986412000
H	-1.671329000	3.717301000	-0.542024000
H	-1.094823000	4.769511000	-1.851633000
H	-0.335494000	4.858348000	-0.248266000
C	-0.330951000	1.912526000	-2.985096000
H	0.382764000	1.223306000	-3.461169000
H	-0.679867000	2.616800000	-3.756994000
H	-1.183010000	1.316231000	-2.630592000
C	1.918804000	3.833126000	-2.360576000
H	2.402340000	4.512345000	-1.644037000
H	1.558561000	4.434040000	-3.210374000
H	2.686990000	3.142494000	-2.742512000
C	2.772477000	-0.294128000	-2.854447000

H	2.029588000	-0.769516000	-3.514402000
H	3.717178000	-0.212787000	-3.414357000
H	2.425700000	0.725730000	-2.634986000
C	4.288210000	-0.408393000	-0.202453000
H	4.479059000	-0.932596000	0.744789000
H	3.970131000	0.615767000	0.039611000
H	5.243137000	-0.338975000	-0.747233000
C	3.880398000	-2.907289000	-1.879307000
H	4.166234000	-3.578463000	-1.056284000
H	4.797337000	-2.639440000	-2.427529000
H	3.231504000	-3.470078000	-2.568113000
C	3.029306000	-3.047859000	1.822178000
H	3.945023000	-3.156246000	1.223296000
H	3.001527000	-3.873571000	2.550040000
H	3.105504000	-2.105798000	2.388697000
C	1.376838000	-4.715725000	-0.177968000
H	0.404141000	-4.813726000	-0.686338000
H	1.475332000	-5.564210000	0.517045000
H	2.164567000	-4.801757000	-0.937858000
C	0.042722000	-3.208762000	2.043544000
H	0.243831000	-2.617017000	2.948637000
H	-0.030093000	-4.260963000	2.361579000
H	-0.940411000	-2.909354000	1.652632000
C	-3.734651000	0.790749000	0.235725000
C	-2.912736000	1.762956000	1.098415000
H	-2.749265000	1.355279000	2.109109000
H	-3.457362000	2.715075000	1.201462000
H	-1.933406000	1.978173000	0.645914000
C	-4.082757000	1.448489000	-1.098848000
H	-3.174502000	1.666993000	-1.681047000
H	-4.605544000	2.400727000	-0.913500000
H	-4.748415000	0.817405000	-1.705735000
C	-4.994220000	0.407034000	1.021955000
H	-5.708087000	-0.171306000	0.423519000
H	-5.503345000	1.327618000	1.348262000
H	-4.744165000	-0.171014000	1.925703000
C	-3.235960000	-1.987519000	-1.109759000
C	-3.019782000	-1.554300000	-2.563680000
H	-3.589390000	-0.650488000	-2.818557000
H	-3.354324000	-2.365955000	-3.229491000
H	-1.958290000	-1.353273000	-2.760470000
C	-4.709832000	-2.307946000	-0.853820000
H	-4.913704000	-2.503986000	0.210214000
H	-4.980484000	-3.213895000	-1.418731000
H	-5.367551000	-1.496281000	-1.194997000
C	-2.385124000	-3.234433000	-0.827385000
H	-1.309448000	-3.010907000	-0.906914000
H	-2.622171000	-4.015457000	-1.567059000
H	-2.581174000	-3.640481000	0.176071000
H	0.697153000	0.111790000	3.379385000
C	-0.336362000	-0.145906000	3.079514000
O	-0.472403000	-0.286118000	1.753136000
O	-1.249100000	-0.286634000	3.834705000

TS8-4: E= -2879.0698526

P	-2.556922000	-1.048867000	-0.055159000
H	-1.938658000	-0.600381000	2.063849000
Si	1.121422000	2.676233000	1.482001000
Si	0.516930000	2.900096000	-1.684899000
Si	3.429460000	-1.065516000	-1.049832000
Si	1.836114000	-2.711226000	1.152678000

Al	0.521457000	0.018840000	-0.210101000
O	-1.151701000	-0.312496000	-0.472715000
C	1.106265000	1.870362000	-0.216760000
H	2.187903000	1.734585000	-0.412562000
C	1.752439000	-1.496395000	-0.299261000
H	1.249750000	-2.091891000	-1.092377000
C	-0.591987000	3.207488000	2.061804000
H	-0.920235000	4.135277000	1.572578000
H	-0.583720000	3.385217000	3.148714000
H	-1.333882000	2.427353000	1.842170000
C	2.256671000	4.184975000	1.473413000
H	3.270791000	3.912152000	1.141966000
H	2.334590000	4.625969000	2.479146000
H	1.876172000	4.962976000	0.793243000
C	1.815684000	1.412304000	2.707742000
H	1.147595000	0.537906000	2.787957000
H	1.922999000	1.840114000	3.716681000
H	2.807977000	1.061730000	2.381833000
C	-0.748340000	4.223464000	-1.230508000
H	-1.649929000	3.808759000	-0.758016000
H	-1.057884000	4.751168000	-2.146194000
H	-0.316296000	4.969572000	-0.545851000
C	-0.242795000	1.780512000	-3.005342000
H	0.502718000	1.078925000	-3.413395000
H	-0.645547000	2.365871000	-3.845952000
H	-1.060103000	1.185317000	-2.570040000
C	2.006934000	3.790435000	-2.430259000
H	2.468905000	4.462468000	-1.690752000
H	1.705204000	4.395645000	-3.299122000
H	2.777599000	3.080235000	-2.766662000
C	3.163136000	-0.203790000	-2.712233000
H	2.525225000	-0.812894000	-3.372503000
H	4.124517000	-0.045195000	-3.224768000
H	2.686740000	0.781136000	-2.591400000
C	4.479658000	0.066690000	0.040052000
H	4.652319000	-0.368002000	1.034514000
H	4.034723000	1.063134000	0.178724000
H	5.461060000	0.208690000	-0.439292000
C	4.441527000	-2.621948000	-1.401012000
H	4.704344000	-3.165050000	-0.481193000
H	5.378389000	-2.352922000	-1.912850000
H	3.884429000	-3.311085000	-2.054606000
C	3.316688000	-2.396473000	2.282143000
H	4.284706000	-2.534371000	1.778668000
H	3.271512000	-3.107512000	3.121924000
H	3.286273000	-1.379729000	2.703311000
C	1.959249000	-4.473376000	0.482571000
H	1.066646000	-4.736504000	-0.105443000
H	2.035212000	-5.189546000	1.315482000
H	2.839990000	-4.604199000	-0.162036000
C	0.321154000	-2.632714000	2.272976000
H	0.326727000	-1.722537000	2.889372000
H	0.329469000	-3.498021000	2.954798000
H	-0.628886000	-2.654807000	1.717604000
C	-3.848909000	0.249669000	-0.508394000
C	-3.358054000	1.539074000	0.162721000
H	-3.302035000	1.424716000	1.255908000
H	-4.068885000	2.354838000	-0.046464000
H	-2.367924000	1.831849000	-0.215561000
C	-4.069801000	0.523355000	-1.996074000
H	-3.138204000	0.816258000	-2.501254000

H	-4.782123000	1.357686000	-2.106380000
H	-4.494694000	-0.341734000	-2.523203000
C	-5.163666000	-0.169441000	0.164450000
H	-5.588769000	-1.083514000	-0.272797000
H	-5.906984000	0.634950000	0.043201000
H	-5.014365000	-0.333645000	1.242427000
C	-2.614142000	-2.458793000	-1.308503000
C	-2.081261000	-2.062619000	-2.687035000
H	-2.714223000	-1.322214000	-3.189647000
H	-2.033469000	-2.957527000	-3.329192000
H	-1.066058000	-1.645306000	-2.610699000
C	-4.032436000	-3.027800000	-1.400720000
H	-4.441172000	-3.256219000	-0.403401000
H	-4.011358000	-3.967985000	-1.975039000
H	-4.724789000	-2.343101000	-1.909501000
C	-1.689767000	-3.538409000	-0.727215000
H	-0.669804000	-3.148921000	-0.588760000
H	-1.633636000	-4.394174000	-1.419515000
H	-2.052289000	-3.904042000	0.245406000
H	-1.518166000	1.154454000	4.265776000
C	-2.135604000	0.554902000	3.567715000
O	-1.371630000	-0.041501000	2.660267000
O	-3.328710000	0.465137000	3.625822000

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