Electronic Supplementary Information

Synthesis of a monomolecular anionic FLP complex

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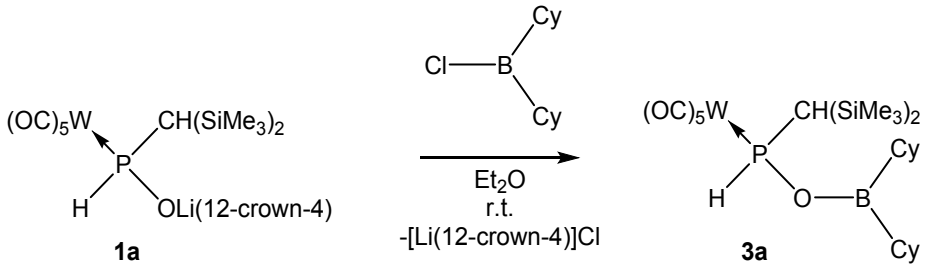
Experimental section

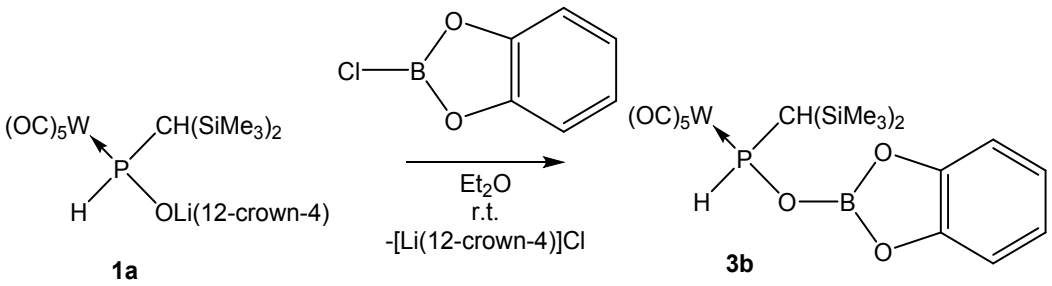
General procedures. All operations were performed under an argon atmosphere, using common Schlenk techniques and dry solvents. Tetrahydrofuran, diethyl ether and *n*-pentane were dried over sodium wire/benzophenone and further purified by subsequent distillation. All NMR spectra were recorded on a Bruker AX-300 spectrometer (300.1 MHz for ^{1}H, 96.25 MHz for ^{11}B, 75.5 MHz for ^{13}C, 59.6 MHz for ^{29}Si and 121.5 MHz for ^{31}P). The ^{1}H and ^{13}C NMR spectra were referenced to the residual proton resonances and the ^{13}C NMR signals of the deuterated solvents, ^{11}B to 15% $BF_3.OEt_2$ in $CDCl_3$ and ^{31}P to 85% H_3PO_4 as external standard, respectively. Melting points were determined in one-side melted off capillaries using a Büchi Type S or a Carl Roth Type MPM-2 apparatus, which are uncorrected. Elemental analyses were carried out on a Vario EL gas chromatograph. Mass spectrometric data were collected on a Kratos MS 50 spectrometer using EI, 70 eV. IR spectra of all compounds were recorded on a Thermo IR spectrometer with an attenuated total reflection (ATR) attachment. The X-ray analyses were performed on a Bruker APEX-II CCD, Bruker X8-KappaApexII or Bruker D8-Venture type diffractometer at 100 or 123 K. The structures were solved by direct methods refined by full-matrix least-squares technique in anisotropic approximation for non-hydrogen atoms using SHELXS97 and SHELXL97[1] program packages. Hydrogen atoms were located from Fourier synthesis and refined isotropically. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary publication no. CCDC-1497789 (**3a**), CCDC-1470387 (**6**) which can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.



Preparation of 3a. In a Schlenk tube, 714.48 mg (1.0 mmol) of complex **1a** were dissolved in 5 mL of diethyl ether, and 1.0 mL (1.0 mmol, 1.0 M in *n*-hexane) of dicyclohexylchloroborane was added. After 5 hours the reaction was completed (checked by ^{31}P NMR), all volatiles were removed in vacuo (~ 2 $\cdot 10^{-2}$ mbar). The crude mixture was extracted four times with 2 mL of *n*-pentane and the solvent was removed *in vacuo* (~ 2 $\cdot 10^{-2}$ mbar) to yield **3a** as white powder.

Complex 3a: Yield: (0.525 g, 0.743 mmol, 74 %). ^{1}H NMR (300.1 MHz, C_6D_6, 25 °C, ppm): δ = 0.07 (s, 9 H, Si(CH_3)$_3$), 0.31 (s, 9 H, Si(CH_3)$_3$), 1.05 (dd, 1 H, $^{2}J_{P,H}$ = 2.9 Hz, $^{3}J_{H,H}$ = 2.9 Hz C*H*), 1.09 – 1.84 (m, 22 H, CH_2), 8.35 (dd, 1 H, $^{1}J_{P,H}$ = 330.9 Hz, $^{3}J_{H,H}$ = 2.9 Hz, P*H*); ^{11}B{^{1}H} NMR (96.25 MHz, C_6D_6, 25 °C): δ = 52.2 (s). ^{13}C{^{1}H} NMR (75.5 MHz, C_6D_6, 25 °C, ppm): δ = 0.4 (d, $^{3}J_{P,C}$ = 2.9 Hz, Si(*C*H$_3$)$_3$), 2.6 (d, $^{3}J_{P,C}$ = 2.9 Hz, Si(*C*H$_3$)$_3$), 25.8 (d, $^{1}J_{P,C}$ = 10.3 Hz, P-*C*), 27.1 – 28.6 (10x CH_2), 30.8 (s, B-*C*H), 197.4 (d_{sat}, $^{1}J_{W,P}$ = 125.8 Hz, $^{2}J_{P,C}$ = 7.8 Hz, *cis*-*C*O), 199.3 (d, $^{2}J_{P,C}$ = 26.5 Hz, *trans*-*C*O); ^{29}Si (59.6 MHz, C_6D_6, 25°C, ppm) δ = 0.0 (d, $^{2}J_{P,Si}$ = 6.1 Hz, *Si*(CH$_3$)$_3$),

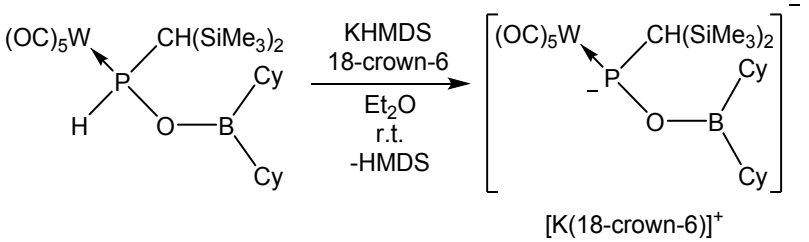
1.4 (d, $^{2}J_{P,Si}$ = 7.6 Hz, *Si*$(CH_3)_3$); ^{31}P NMR (121.5 MHz, $CDCl_3$, 25 °C, ppm): δ = 81.5 (d_{sat}, $^{1}J_{W,P}$ = 277.9 Hz, $^{1}J_{P,H}$ = 330.9 Hz); IR (ATR, ũ [cm^{-1}]): ũ = 2311 (w, ν(PH)), 2070 (m, ν(CO)), 1982 (w, ν(CO)), 1933 (vs, ν(CO)), 1911 (vs, ν(CO)). MS (EI, 60 eV, m/z (%)): 708.1 (26) [M] $^{\bullet+}$, 680.1 (22) [M-1 CO] $^{+}$; EA [%]: calculated: C: 40.69, H: 5.98, found: C: 40.09, H: 5.96; Melting Point: 96 °C.



1a **3b**

Preparation of 3b. In a Schlenk tube, 357.2 mg (0.5 mmol) of complex **1a** were dissolved in 2 mL of diethyl ether and a solution of 77,18 mg (0.5 mmol) catecholchloroborane in 2 mL diethyl ether was added. After 5 hours the reaction was completed (checked by ^{31}P NMR), all volatiles were removed in vacuo (~ 2 ·10^{-2} mbar). The crude mixture was extracted four times with 1 mL of *n*-pentane and the solvent was removed *in vacuo* (~ 2 ·10^{-2} mbar) to yield **3b** as white powder.

Complex 3b: Yield: (0.255 g, 0.39 mmol, 78 %). ^{1}H NMR (300.1 MHz, C_6D_6, 25 °C, ppm): δ = -0.03 (s, 9 H, Si-C*H*$_3$), 0.28 (s, 9 H, Si-C*H*$_3$), 0.98 (dd, 1 H, $^{2}J_{P,H}$ = 3.2 Hz, $^{3}J_{H,H}$ = 2.3 Hz C*H*), 6.66 – 6.72 (m, 2 H, Ar-*H*), 6.87 – 6.94 (m, 2 H, Ar-*H*), 8.46 (dd, 1 H, $^{1}J_{P,H}$ = 341.8 Hz, $^{3}J_{H,H}$ = 2.3 Hz, P*H*). ^{11}B{^{1}H} NMR (96.25 MHz, C_6D_6, 25 °C, ppm): δ = 21.7 (s); ^{13}C{^{1}H} NMR (75.5 MHz, C_6D_6, 25 °C, ppm): δ = 0.0 (d, $^{3}J_{P,C}$ = 2.9 Hz, Si(*C*H$_3$)$_3$), 2.2 (d, $^{3}J_{P,C}$ = 3.2 Hz, Si(*C*H$_3$)$_3$), 25.2 (d, $^{1}J_{P,C}$ = 11.0 Hz, P-*C*), 112.7 (s, Ph-*C*H), 123.3 (s, Ph-*C*H), 148.0 (s, Ph-*C*), 196.6 (d_{sat}, $^{1}J_{W,C}$ = 126.1 Hz, $^{2}J_{P,C}$ = 7.4 Hz, *cis*-CO), 199.2 (d, $^{2}J_{P,C}$ = 27.8 Hz, *trans*-CO); ^{29}Si (59.6 MHz, C_6D_6, 25°C, ppm) δ = 1.0 (d, $^{2}J_{P,Si}$ = 6.1 Hz, *Si*$(CH_3)_3$), 1.9 (d, $^{2}J_{P,Si}$ = 8.7 Hz, *Si*$(CH_3)_3$); ^{31}P NMR (121.5 MHz, C_6D_6, 25 °C, ppm): δ = 97.7 (d, $^{1}J_{P,H}$ = 331.6 Hz, $^{1}J_{W,P}$ = 277.1 Hz); IR (ATR, ũ [cm^{-1}]): ũ = 2300 (w, ν(PH)), 2075 (m, ν(CO)), 1986 (w, ν(CO)), 1944 (w, ν(CO)), 1912 (vs, ν(CO)); MS (EI, 60 eV, m/z (%)): 650.0 (15) [M] $^{\bullet+}$, 622.0 (5) [M-1 CO] $^{+}$, 594.0 (55) [M - 2 CO] $^{+}$, 73.1 (100) [$SiMe_3$]$^{+}$; EA [%]: calculated: C: 33.25, H: 3.72, found: C: 33.49, H: 3.97; Melting Point: 114°C.

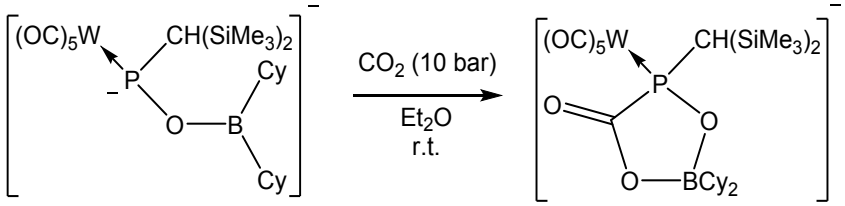


2a **5**

Preparation of 5. In a Schlenk tube, 141.3 mg (0.2 mmol) of complex **3a** were dissolved in 5 mL of diethyl ether, and a solution of 39.9 mg (0.2 mmol) KHMDS and 52.86 mg (0.2 mmol) 18-crown-6 in 10 mL diethyl ether was added dropwise. The volatiles were

removed 20 Minutes after finishing the addition of the KHMDS solution. The crude mixture was washed four times with 2 mL of *n*-pentane and the solvent was removed *in vacuo* (~ 2 $\cdot 10^{-2}$ mbar) to yield **5** as an orange powder.

Complex 5: Yield: (0.149 g, 0.15 mmol, 75 %). ^{1}H NMR (300.1 MHz, THF-d_8, 25 °C, ppm): δ = 0.07 (d, 9 H, $^{3}J_{P,C}$ = 1.6 Hz, Si(CH_3)$_3$), 0.19 (s, 9 H, Si(CH_3)$_3$), 2.09 (s, 1 H, P-C*H*), 1.18 – 1.68 (m, 22 H, CH_2); ^{11}B{^{1}H} NMR (96.25 MHz, C_6D_6, 25 °C, ppm): δ = 51.7 (s); ^{13}C{^{1}H} NMR (75.5 MHz, THF-d_8, 25 °C): δ = 1.1 (d, $^{3}J_{P,C}$ = 13.6 Hz, Si(*C*H$_3$)$_3$), 4.2 (s, Si(*C*H$_3$)$_3$), 25.2 (d, $^{1}J_{P,C}$ = 73.3 Hz, P-*C*), 28.2 – 28.9 (10x CH$_2$), 31.8 (s, B-*C*H), 207.2 (d$_{sat}$, $^{1}J_{W,P}$ = 127.8 Hz, $^{2}J_{P,C}$ = 5.6 Hz, *cis*-*C*O), 210.9 (d, $^{1}J_{W,P}$ = 153.6 Hz, $^{2}J_{P,C}$ = 15.1 Hz, *trans*-*C*O); ^{29}Si (59.6 MHz, THF-d_8, 25°C, ppm) δ = -5.9 (d, $^{2}J_{P,Si}$ = 32.2 Hz, *Si*(CH$_3$)$_3$), -2.0 (d, *Si*(CH$_3$)$_3$); ^{31}P NMR (121.5 MHz, THF-d_8, 25 °C, ppm): δ = 190.2 (s$_{sat}$, $^{1}J_{W,P}$ = 71.8 Hz); IR (ATR, $\tilde{\upsilon}$ [cm^{-1}]): $\tilde{\upsilon}$ = 2028 (m, ν(CO)), 1929 (w, ν(CO)), 1901 (s, ν(CO)), 1873 (vs, ν(CO)), 1844 (vs, ν(CO)); MS (ESI, negative, m/z (%)): 707.2 (50) [M]$^{\bullet-}$, 678.9 (12) [M- 1 CO]$^{-}$, 623.1 (55) [M - 3 CO]$^{-}$, (ESI, positive, m/z (%)): 303.1 (100) [M]$^{\bullet+}$; Melting Point: 85°C.

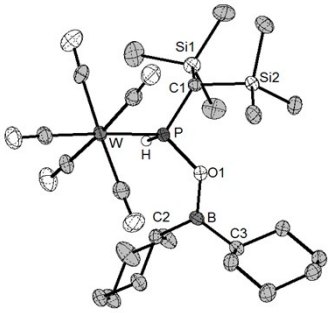


[K(18-crown-6)]$^{+}$ **5** [K(18-crown-6)]$^{+}$ **6**

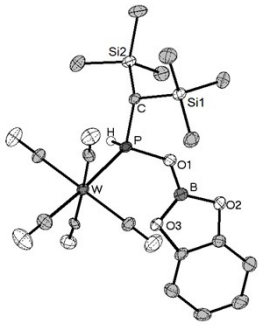
Preparation of 6. In a Schlenk tube, 112.5 mg (0.11 mmol) of complex **5** were dissolved in 7 mL of diethyl ether. This solution was stirred for 18 hours under 1 bar of CO_2 atmosphere. After the removal of all volatiles, the crude mixture was washed four times with 1 mL of *n*-pentane and the solvent was removed *in vacuo* (~ 2 $\cdot 10^{-2}$ mbar) to yield **6** as withe powder.

Complex 6: Yield: (0.071 g, 0.067 mmol, 61 %). ^{1}H NMR (300.1 MHz, THF-d_8, 25 °C, ppm): δ = 0.25 (s, 9 H, Si(CH_3)$_3$), 0.36 (s, 9 H, Si(CH_3)$_3$), 1.01 – 1.66 (m, 22 H, CH_2), 1.27 (d, 1 H, $^{2}J_{P,H}$ = 2.4 Hz, P-C*H*), 3.62 (s, 24 H, crown-CH_2). ^{11}B{^{1}H} NMR (96.25 MHz, THF-d_8, 25 °C, ppm): δ = 13.7 (s); ^{13}C{^{1}H} NMR (75.5 MHz, THF-d_8, 25 °C, ppm): δ = 3.0 (d, $^{3}J_{P,C}$ = 1.6 Hz, Si(*C*H$_3$)$_3$), 3.1 (d, $^{3}J_{P,C}$ = 2.8 Hz, Si(*C*H$_3$)$_3$), 29.0 – 31.5 (10x CH$_2$), 34.6 (d, $^{2}J_{P,C}$ = 6.0 Hz, P-*C*H), 37.2 (d, $^{1}J_{P,C}$ = 118.5 Hz, *C*H-Cy), 71.1 (s, crown), 183.6 (d, $^{1}J_{P,C}$ = 42.4 Hz, P-*C*O), 199.7 (d$_{sat}$, $^{1}J_{W,P}$ = 126.4 Hz, $^{2}J_{P,C}$ = 8.3 Hz, *cis*-*C*O), 202.9 (d, $^{2}J_{P,C}$ = 21.8 Hz, $^{1}J_{W,P}$ = 140.8 Hz, *trans*-*C*O); ^{29}Si (59.6 MHz, THF-d_8, 25°C, ppm) δ = -2.4 (d, $^{2}J_{P,Si}$ = 11.2 Hz, *Si*(CH$_3$)$_3$), -0.6 (d, $^{2}J_{P,Si}$ = 5.9 Hz *Si*(CH$_3$)$_3$). ^{31}P NMR (121.5 MHz, THF-d_8, 25 °C, ppm): δ = 89.6 (d$_{sat}$, $^{1}J_{W,P}$ = 272.6 Hz, $^{2}J_{P,H}$ = 2.4 Hz); IR (ATR, $\tilde{\upsilon}$ [cm^{-1}]): $\tilde{\upsilon}$ = 2064 (m, ν(CO)), 1973 (w, ν(CO)), 1921 (s, ν(CO)), 1897 (s, ν(CO)), 1656 (m, ν(CO)); MS (ESI, positive, m/z (%)): 751.2 (100) [M]$^{\bullet-}$, 707.2 (55) [M- CO_2]$^{\bullet-}$; (ESI, negative, m/z (%)): 303.1 (100) [M]$^{\bullet+}$; EA [%]: calculated: C: 42.13, H: 6.21, found: C: 43.28, H: 6.54; Decomposition Point: 163 °C.

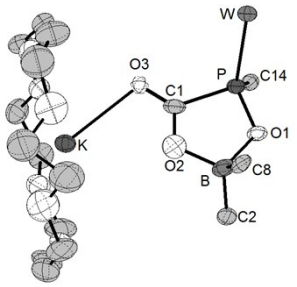
Crystal data and summary of data collection and refinement



Crystal Data for 3a: Suitable single-crystals of **3a** were obtained from a concentrated *n*-pentane solution at -30 °C. Data were collected with a with a Bruker APEX-II CCD diffractometer equipped with a low-temperature device at 100 K by using graphite monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by Patterson methods (SHELXS-97)[1] and refined by full-matrix least-squares on F^2 (SHELXL-97)[1] $C_{24}H_{42}BO_6PSi_2W$, M = 708.38, crystal dimensions 0.18 × 0.17 × 0.05 mm^3, monoclinic, space group C 2/c, Z = 8, a = 19.042(6) Å, b = 9.093(3) Å, c = 35.451(11) Å, α = 90.0°, β = 94.657(5)°, γ = 90.0°, V = 6118.0(3) $Å^3$, d_c = 1.538 g cm^{-3}, μ = 3.940 mm^{-1}, T = 100 K, transmission factors (min./max.) 0.501/ 0.746, empirical absorption correction, 2θmax= 55.998°, no. of unique data 7330, Rint = 0.0878, R1 (for I > 2σ(I)) = 0.0433, wR2 (for all data) = 0.1087, final R = 0.0569, goodness of fit 1.023, ΔF(max./min.) = 1.01/ -2.13 e $Å^{-3}$.



Crystal Data for 2b: Suitable single-crystals of **3b** were obtained from a concentrated *n*-pentane solution at -30 °C. Data were collected with a with a Nonius KappaCCD diffractometer equipped with a low-temperature device at 123 K by using graphite monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by Patterson methods (SHELXS-97)[1] and refined by full-matrix least-squares on F^2 (SHELXL-97)[1] $C_{18}H_{24}BO_8PSi_2W$, M = 650.18, crystal dimensions 0.34 × 0.16 × 0.1 mm^3, triclinic, space group P -1, Z = 2, a = 8.7638(3) Å, b = 11.0103(4) Å, c = 14.5026(6) Å, α = 108.2413(19)°, β = 105.4429(17)°, γ = 91.170(2)°, V = 1272.82(8) $Å^3$, d_c = 1.696 g cm^{-3}, μ = 4.733 mm^{-1}, T = 123 K, transmission factors (min./max.) 0.3464/ 0.6657, empirical absorption correction, 2θmax= 56.0°, no. of unique data 5900, Rint = 0.0610, R1 (for I > 2σ(I)) = 0.0329, wR2 (for all data) = 0.0778, final R = 0.0371, goodness of fit 1.013, ΔF(max./min.) = 2.37/ -2.35 e $Å^{-3}$.



Crystal Data for 6: Suitable single-crystals of **6** were obtained from a concentrated *n*-pentane solution at 4 °C. Data were collected with a with a Bruker D8-Venture diffractometer equipped with a low-temperature device at 123 K by using graphite monochromated CuKα radiation (λ = 1.54178 Å). The structure was solved by Patterson methods (SHELXS-97)[1] and refined by full-matrix least-squares on F^2 (SHELXL-97)[1] $C_{79}H_{142}B_2K_2O_{28}P_2Si_4W_2$, M = 2181.74, crystal dimensions 0.1 × 0.03 × 0.02 mm^3, monoclinic, space group $P2_1/c$, Z = 2, a = 10.9829(3) Å, b = 19.8205(6) Å, c = 24.0592(8) Å, α = 90°, β = 96.5137(17)°, γ = 90°, V = 5203.6(3) $Å^3$, d_c = 1.392 g cm^{-3}, μ = 6.028 mm^{-1}, T = 123 K, transmission factors (min./max.) 0.5693/ 0.7536, empirical absorption correction, 2θmax= 135.49°, no. of unique data 9282, Rint = 0.0991, R1 (for I > 2σ(I)) = 0.0560, wR2 (for all data) = 0.1415, final R = 0.0864, goodness of fit 1.029, ΔF(max./min.) = 1.58/ -1.01 e $Å^{-3}$.

Literature

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3. DFT calculations

Computational Details: The quantum chemical DFT calculations have been performed with the TURBOMOLE 7.0 suite of programs.[1] The structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO (Et_2O) level of theory, which combines the TPSS functional[2] with the BJ-damped D3-dispersion[3] and def2-TZVP basis set[4] as well as the Conductor-like Screening Model (COSMO) continuum solvation model[5] for Et_2O solvent (dielectric constant ε = 4.34, refractive constant n = 1.352, and effective radius R_{solv} = 3.46 Å). The density-fitting RI-J approach[6] is used to accelerate the geometry optimization and numerical harmonic frequency calculations in solution. The fully optimized structures are characterized by frequency analysis to identify the nature of located stationary points (no imaginary frequency for true minima and only one imaginary frequency for transition state) and to provide thermal enthalpy and free-energy corrections according to the modified ideal gas–rigid rotor–harmonic oscillator model.[7]

The final solvation energies in toluene are computed with the more reliable COSMO-RS solvation model (parameter file: BP_TZVP_C30_1301.ctd) implemented in the COSMOtherm (Version C3.0 Release 14.01) program package[8] on the above TPSS-D3 optimized structures. Single-point calculations using the meta-GGA TPSS-D3 functionals are performed using a large def2-QZVP basis set.[9] Test calculations using larger diffuse augmented def2-QZVPD basis set[10] turn out to have very small effects on reaction energies as compared with those using the def2-QZVP basis set, with the respective mean and standard deviations being only 0.2 and 0.3 kcal/mol, and thus are not discussed further. The final reaction enthalpies (ΔH) and Gibbs free energies (ΔG) are determined from the gas-phase single-point energies plus the corresponding thermal and COSMO-RS solvation corrections. In our discussion, the more reliable PW6B95-D3 final Gibbs free energies (in kcal/mol, at 298.15 K and 1 bar gas and 1 mol/L concentration in solution as standard states) will be used unless specified otherwise.

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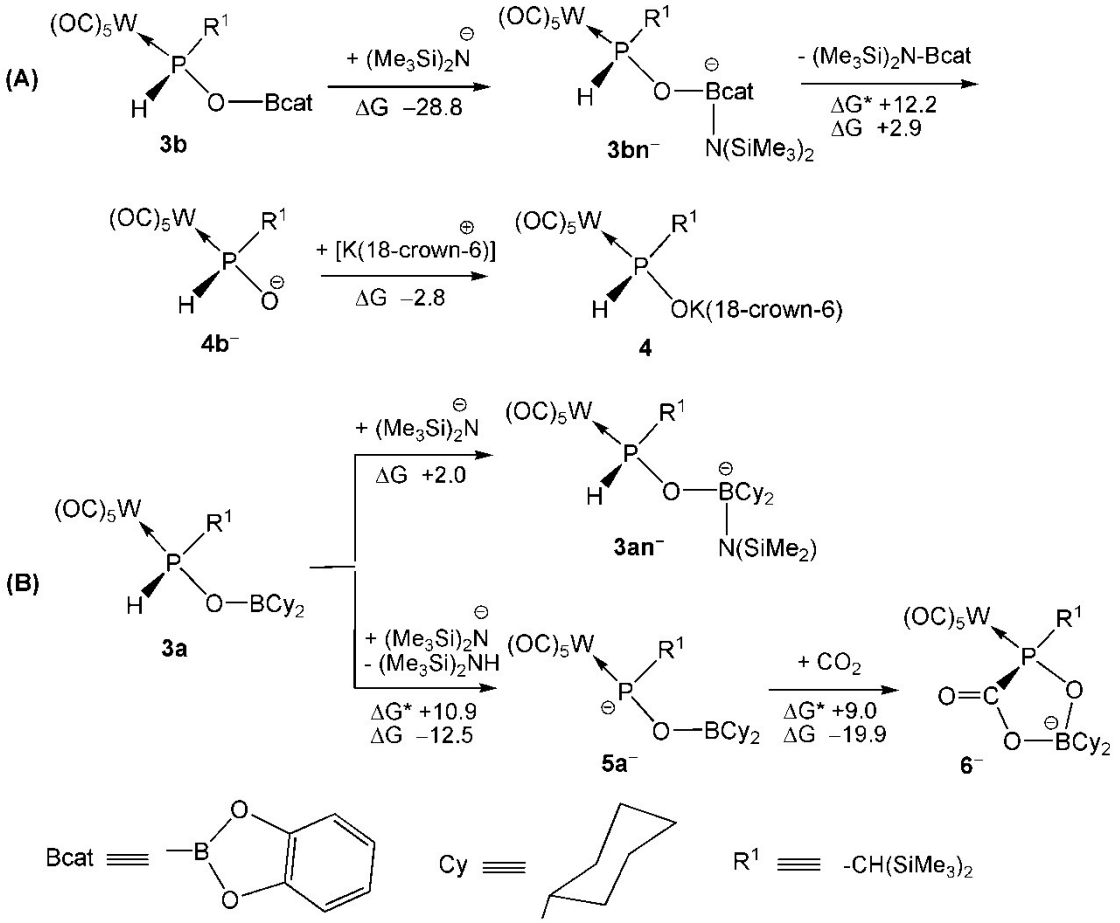

Figure S1. Detailed reaction free energy paths (in kcal/mol) at the TPSS-D3 + COSMO-RS (Et_2O) level of theory.

Table S1. The TPSS-D3/def2-TZVP + COSMO (Et_2O) computed lowest imaginary frequency (ImF), gas-phase enthalpic (Hc) and Gibbs free-energy (Gc) corrections; the COSMO-RS computed solvation enthalpic (Hsol) and Gibbs free-energy (Gsol) corrections in Et_2O solution; the TPSS-D3 + COSMO total energies (TPSS-D3); the TPSS-D3/def2-QZVP single-point energies (TPSS-D3); the relative electronic energies (Ee), Gibbs free-energies (G) and enthalpies (H) at the TPSS-D3 level. The deviations with respect to TPSS-D3/def2-QZVPD calculations (Diff) are also shown for comparison. Each structure is labeled either by its molecular formula or a specific name in bold, followed by the respective superscript + and – for singly charged cationic and anionic species. Each transition structure (with only one imaginary frequency) is indicated by the "**TS**" prefix.

Species	ImF	Hc	Gc	Hsol	Gsol	COSMO	TPSS-D3	Ee	G	H	Diff
	cm^{-1}	kcal/mol	kcal/mol	kcal/mol	kcal/mol	E_h	E_h	kcal/mol	kcal/mol	kcal/mol	kcal/mol
CO_2	0	9.36	-5.88	0.00	0.00	-188.69773	-188.70543	--	--	--	--
OEt_2	0	89.19	66.09	-6.69	-0.23	-233.79976	-233.81353	--	--	--	--
n$^-$ $N(SiMe_3)_2^-$	0	149.87	112.68	-50.73	-43.19	-873.67277	-873.67414	--	--	--	--
nH $HN(SiMe_3)_2$	0	158.59	122.99	-9.49	-2.62	-874.21870	-874.26185	--	--	--	--
na $N(SiMe_3)_2BCy_2$	0	361.55	308.93	-17.93	-9.59	-1369.35397	-1369.42993	--	--	--	--
nb $N(SiMe_3)_2$Bcat	0	214.98	170.76	-15.95	-7.96	-1280.34260	-1280.40440	--	--	--	--
K$^+$ K(18-crown-6)$^+$	0	242.46	198.19	-52.82	-43.73	-1523.45245	-1523.48135	--	--	--	--
K$^+$.OEt_2	0	332.93	276.93	-51.85	-42.74	-1757.27017	-1757.31715	--	--	--	--
K$^+$**.n**$^-$	0	393.90	327.45	-31.50	-21.22	-2397.18206	-2397.28440	--	--	--	--
3b	0	267.56	200.50	-22.14	-12.55	-2315.85567	-2315.95997	--	--	--	--
3bn$^-$	0	419.65	332.52	-49.92	-38.92	-3189.61592	-3189.73769	--	--	--	--
TS34$^-$	-267	418.44	332.91	-50.73	-39.56	-3189.59523	-3189.71792	--	--	--	--
4b$^-$	0	203.45	145.30	-48.13	-39.35	-1909.24106	-1909.28901	--	--	--	--
4	0	447.25	359.29	-34.63	-23.56	-3432.74872	-3432.89489	--	--	--	--
3a	0	415.06	339.76	-23.35	-13.78	-2404.89065	-2405.00901	--	--	--	--
3an$^-$	0	567.16	474.48	-50.23	-38.93	-3278.60806	-3278.74388	--	--	--	--
3a.n$^-$	0	566.81	471.18	-52.22	-40.64	-3278.55513	-3278.72256	--	--	--	--

TS45^{-}	-698	564.46	470.36	-51.43	-39.94	-3278.58374	-3278.72145	--	--	--	--
5a^{-}	0	407.37	332.00	-51.98	-41.64	-2404.37761	-2404.46564	--	--	--	--
5a^{-}.$HN(SiMe_3)_2$	0	568.37	471.76	-52.69	-41.05	-3278.61211	-3278.74761	--	--	--	--
5	0	652.29	547.43	-43.09	-30.75	-3927.86512	-3928.04329	--	--	--	--
5a^{-}.CO_2	0	417.76	336.78	-52.26	-41.85	-2593.08215	-2593.17903	--	--	--	--
TS56^{-}	-106	417.23	338.44	-52.02	-41.70	-2593.07958	-2593.17632	--	--	--	--
6a^{-}	0	418.38	340.51	-54.15	-43.59	-2593.12694	-2593.22252	--	--	--	--
6	-8	661.43	556.77	-43.20	-30.71	-4116.63297	-4116.82128	--	--	--	--
K^+ + OEt_2	0	331.65	264.28	-59.51	-43.96	-1757.25221	-1757.29488	0.0	0.0	0.0	0.0
K^+.OEt_2	0	332.93	276.93	-51.85	-42.74	-1757.27017	-1757.31715	-14.0	-0.1	-5.0	0.1
K^+ + **n**$^{-}$	0	392.33	310.87	-103.55	-86.91	-2397.12522	-2397.15550	0.0	0.0	0.0	0.0
K^+**.n**$^{-}$	0	393.90	327.45	-31.50	-21.22	-2397.18206	-2397.28440	-80.9	1.4	-7.3	0.6
K^+ + **4b**$^{-}$	0	445.91	343.49	-100.95	-83.08	-3432.69351	-3432.77037	0.0	0.0	0.0	0.0
4	0	447.25	359.29	-34.63	-23.56	-3432.74872	-3432.89489	-78.1	-2.8	-10.5	0.1
K^+ + **5a**$^{-}$	0	649.83	530.19	-104.80	-85.36	-3927.83006	-3927.94699	0.0	0.0	0.0	0.0
5	0	652.29	547.43	-43.09	-30.75	-3927.86512	-3928.04329	-60.4	11.4	3.7	-0.4
K^+ + **6a**$^{-}$	0	660.84	538.71	-106.97	-87.32	-4116.57939	-4116.70387	0.0	0.0	0.0	0.0
6	-8	661.43	556.77	-43.20	-30.71	-4116.63297	-4116.82128	-73.7	1.0	-9.3	0.2
3b + **n**$^{-}$	0	417.43	313.17	-72.86	-55.73	-3189.52844	-3189.63412	0.0	0.0	0.0	0.0
3bn^{-}	0	419.65	332.52	-49.92	-38.92	-3189.61592	-3189.73769	-65.0	-28.8	-39.8	0.5
TS34^{-}	-267	418.44	332.91	-50.73	-39.56	-3189.59523	-3189.71792	-52.6	-16.7	-29.4	0.5
4a^{-} + **nb**	0	418.43	316.06	-64.08	-47.31	-3189.58366	-3189.69341	-37.2	-25.9	-27.4	0.5

3a + **n**$^{-}$	0	564.94	452.43	-74.08	-56.96	-3278.56342	-3278.68316	0.0	0.0	0.0	0.0
3an^{-}	0	567.16	474.48	-50.23	-38.93	-3278.60806	-3278.74388	-38.1	2.0	-12.0	0.6
4b^{-} + **na**	0	565.00	454.22	-66.05	-48.94	-3278.59502	-3278.71894	-22.5	-12.6	-14.4	0.5
3a.n^{-}	0	566.81	471.18	-52.22	-40.64	-3278.55513	-3278.72256	-24.7	10.4	-1.0	0.5
TS45^{-}	-698	564.46	470.36	-51.43	-39.94	-3278.58374	-3278.72145	-24.0	10.9	-1.9	0.6
5a^{-}.$HN(SiMe_3)_2$	0	568.37	471.76	-52.69	-41.05	-3278.61211	-3278.74761	-40.4	-5.2	-15.6	0.4
5a^{-} + **nH**	0	565.96	454.99	-61.48	-44.25	-3278.59630	-3278.72749	-27.8	-12.5	-14.2	0.5
5a^{-} + CO_2	0	416.73	326.12	-51.98	-41.64	-2593.07534	-2593.17106	0.0	-12.5	0.0	0.0
5a^{-}.CO_2	0	417.76	336.78	-52.26	-41.85	-2593.08215	-2593.17903	-5.0	-7.1	-4.3	0.0
TS56^{-}	-106	417.23	338.44	-52.02	-41.70	-2593.07958	-2593.17632	-3.3	-3.6	-2.9	0.0
6a^{-}	0	418.38	340.51	-54.15	-43.59	-2593.12694	-2593.22252	-32.3	-32.4	-32.8	-0.1

Table S2. The TPSS-D3/def2-TZVP + COSMO (Et_2O) optimized atomic Cartesian coordinates (in Å). Each structure is labeled either by its molecular formula or a name in bold (see **Table S1**), followed by the number of atoms, the total energy, and the detailed atomic coordinates (double-column list).

3a.n⁻.xyz
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Energy = -3278.555125255

B	0.4511976	-1.6077514	-0.8865856
O	-0.6025252	-1.2575661	-0.0525067
C	1.0139091	-0.6549110	-2.0148094
C	0.9853005	-3.1028486	-0.7441174
P	-1.5123790	0.1351109	0.0792336
C	0.3049288	-1.0522690	-3.3422041
C	2.5409827	-0.7732281	-2.2199930
H	0.7879038	0.3996995	-1.7909496
C	-0.0675863	-4.1231860	-0.2731438
C	2.2480331	-3.2109808	0.1518255
H	1.3105483	-3.4048494	-1.7559309
C	-2.1284945	0.0587992	1.8153873
H	-0.4890471	1.1655576	0.0190570
W	-3.4978291	0.2487698	-1.5470013
C	0.8104874	-0.2414259	-4.5427053
H	-0.7774879	-0.9219059	-3.2437599
H	0.4739254	-2.1227886	-3.5359803
C	3.0360285	0.0615689	-3.4054186
H	2.8046927	-1.8274143	-2.3955882
H	3.0647160	-0.4599997	-1.3113843
C	0.4851701	-5.5538710	-0.2491842
H	-0.9539300	-4.0748371	-0.9153496
H	-0.3989112	-3.8511951	0.7352606
C	2.8031721	-4.6418764	0.1729042
H	3.0220496	-2.5174529	-0.1908084
H	1.9945979	-2.9108299	1.1761911
Si	-1.7965898	1.5618355	2.9581370
Si	-2.0064645	-1.6530704	2.6419416
H	-3.2181363	0.1349267	1.6783488
N	0.9981937	2.4474719	-0.2569674
C	-2.3845189	1.1677179	-3.0313231
C	-5.0571755	0.3506325	-2.8277877
C	-3.0376402	-1.6505823	-2.1861357
C	-4.0111171	2.0692486	-0.7308192
C	-4.7894573	-0.5825480	-0.1956440
C	2.3304995	-0.3515282	-4.7014819
H	0.3020794	-0.5796649	-5.4556821
H	0.5426590	0.8112991	-4.4006808
H	2.8349919	1.1199560	-3.2033674
H	4.1239213	-0.0466250	-3.5111632
C	1.7392495	-5.6483205	0.6292364
H	0.7397997	-5.8606831	-1.2747358
H	-0.2834696	-6.2517043	0.1092947
H	3.1423037	-4.9090038	-0.8390465
H	3.6825237	-4.6938665	0.8287519
C	-1.4209334	3.1110808	1.9863035
C	-0.4325276	1.2503729	4.2239238
C	-3.4148613	1.8663086	3.8918136
C	-2.8792348	-2.9474244	1.5847942
C	-0.2497253	-2.1672448	3.0679812
C	-2.9814157	-1.6137869	4.2652757
Si	0.7521107	3.8068933	-1.2189326
Si	2.2927325	2.0947794	0.7499615
O	-1.8689000	1.6933323	-3.9204559
O	-5.9526104	0.4053148	-3.5678741
O	-2.8116149	-2.7407197	-2.5046143
O	-4.3726422	3.0521484	-0.2394006
O	-5.5868827	-1.0155927	0.5284392
H	2.6689605	0.2720809	-5.5391340
H	2.5985511	-1.3911900	-4.9459857
H	2.1450362	-6.6687022	0.6140523
H	1.4639150	-5.4293810	1.6714416
H	-1.2019490	3.9332040	2.6806204
H	-2.2846983	3.4093512	1.3830048
H	-0.5591653	2.9906336	1.3129568
H	-0.3033828	2.1539810	4.8335658
H	-0.6755575	0.4254839	4.9027986
H	0.5301434	1.0338665	3.7530716
H	-3.3141877	2.7609243	4.5198726
H	-4.2325173	2.0540480	3.1846387
H	-3.7120908	1.0352824	4.5383489
H	-2.5693560	-2.9136616	0.5385615
H	-3.9633782	-2.7973186	1.6262723
H	-2.6682241	-3.9547494	1.9660322
H	-0.2458578	-3.2042254	3.4281606
H	0.4121562	-2.1030497	2.2034932
H	0.1707671	-1.5365253	3.8575878
H	-4.0225392	-1.3108474	4.1054769
H	-2.5444150	-0.9481810	5.0166564
H	-2.9947293	-2.6270876	4.6890226
C	1.5109380	5.4260102	-0.5448745
C	1.4551047	3.6523467	-2.9833737
C	-1.0956600	4.1950750	-1.4401326
C	2.4452647	3.2073673	2.2956537
C	2.1312775	0.3250300	1.4296236
C	4.0201973	2.1963306	-0.0565016
H	2.6033017	5.3549867	-0.4589902
H	1.1166279	5.6562510	0.4531143
H	1.2854376	6.2801189	-1.1995615
H	1.2763734	4.5629210	-3.5725396
H	0.9955857	2.8152655	-3.5221652
H	2.5383637	3.4763743	-2.9589199
H	-1.6712139	3.2798157	-1.6136466

H	-1.2719627	4.8637195	-2.2931954
H	-1.5126148	4.6756015	-0.5476045
H	1.5161725	3.2203821	2.8772946
H	2.6606020	4.2432400	2.0054908
H	3.2532511	2.8723464	2.9620051
H	2.2545736	-0.4181954	0.6333523
H	1.1397417	0.1618365	1.8653814
H	2.8758228	0.0986064	2.2043967
H	4.0874595	1.5669268	-0.9514497
H	4.2354113	3.2270578	-0.3687079
H	4.8178631	1.8873772	0.6343054

3an$^-$.xyz

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Energy = -3278.608055747

B	-2.1326488	0.2420880	0.3400922
P	0.8527937	0.1984111	0.1465109
H	0.8358682	0.2496606	1.5557101
Si	1.6876583	3.1295703	1.2471805
Si	1.4373624	2.6497966	-1.9088268
W	2.6080437	-1.6655228	-0.3586588
O	4.1707038	-0.0779088	-2.6655364
O	1.3676058	-3.4704862	2.0015757
O	4.9186720	-3.8375960	-0.5225939
O	1.2747207	-3.3476834	-2.7536140
O	4.4778064	-0.2049894	1.7967768
O	-0.6524302	0.1022187	-0.2946910
C	2.2189474	2.3014941	2.8594047
C	-1.4405803	-1.1799982	2.4635477
C	-0.7238477	-0.1131724	4.6393608
C	-1.4315736	-1.3094186	3.9912566
C	0.1056718	4.1295142	1.5054614
C	1.6344849	1.8624249	-0.1810497
C	0.8695122	1.4370283	-3.2240983
C	3.0602515	4.3813248	0.8831999
C	0.2355090	4.0977610	-1.8745553
C	3.1236768	3.2972792	-2.4638910
C	-4.5047454	3.4894755	-0.0619800
C	-4.7389024	3.4330700	-1.5762267
C	-3.9907947	2.1390121	0.4554440
C	-3.4536726	3.0143458	-2.2995432
C	1.7547801	-2.7992558	1.1427559
C	4.0655835	-3.0445733	-0.4761055
C	-2.6872613	1.6831912	-0.2246432
C	-2.9001592	1.6918171	-1.7482117
C	1.6617409	-2.7100591	-1.8702244
C	3.7584590	-0.7072711	1.0371575
C	-1.4087771	1.3542993	2.6859243
C	-1.3878789	1.2026168	4.2137220
C	-2.0401769	0.1497677	1.9691762
C	3.5644494	-0.6112264	-1.8319405
H	-0.0643001	4.2891980	2.5767632
H	2.2883384	3.0708652	3.6395863
H	-2.4688170	-1.3482829	4.3582569
H	3.2081251	1.8440360	2.7514822
H	-0.7234260	-0.2071266	5.7336554
H	-1.9968111	-2.0104116	2.0147109
H	0.3299397	-0.1077405	4.3209861
H	-0.4092236	-1.2879802	2.1027636
H	2.6920425	1.5442064	-0.2188662
H	0.1944672	5.1114770	1.0276510
H	-0.1715130	1.1434647	-3.0786490
H	-0.7814577	3.6379628	1.1003791
H	-0.9486060	-2.2484845	4.2950664
H	1.4720826	0.5239421	-3.2417570
H	0.0394248	4.4390104	-2.8987904
H	0.9559799	1.9155063	-4.2084647
H	3.1974349	5.0176852	1.7676128
H	4.0198019	3.8961199	0.6695842
H	-0.7203479	3.8131428	-1.4258328
H	2.8147776	5.0384891	0.0419547
H	3.8503132	2.4831552	-2.5568073
H	0.6348449	4.9476223	-1.3102512
H	3.5398270	4.0467010	-1.7849102
H	3.0204597	3.7627663	-3.4530221
H	-5.4314157	3.7736086	0.4566947
H	-5.0961368	4.4016191	-1.9518993
H	-3.7606921	4.2698096	0.1597467
H	-5.5294264	2.6966001	-1.7860087
H	-3.8640877	2.1811581	1.5441108
H	-2.7061021	3.8094785	-2.1703054
H	-4.7676598	1.3863839	0.2631499
H	-3.6364256	2.9287384	-3.3803691
H	-1.9226518	2.4471582	0.0044214
H	-3.5980779	0.8800116	-1.9985078
H	-1.9561411	2.2650187	2.4197245
H	-1.9567794	1.4512414	-2.2480802
H	-2.4232110	1.2112915	4.5872501
H	-3.0812429	0.1485555	2.3140645
H	-0.8738392	2.0568618	4.6766788
H	1.5301725	1.5315163	3.2169621
H	-0.3821743	1.5160685	2.3399122
N	-2.9829522	-0.9768240	-0.2219070
Si	-4.5338441	-1.4665432	0.4020884
Si	-2.3580221	-2.0624273	-1.4339651
C	-4.6069511	-3.3270823	0.8090657
C	-5.1625963	-0.7706456	2.0557814
C	-5.9542603	-1.0524161	-0.7912459
C	-3.7184507	-2.9051866	-2.4753788
C	-1.3289083	-1.3199607	-2.8254913
C	-1.3508636	-3.4395864	-0.6236629
H	-3.9544287	-3.5295417	1.6683950
H	-5.2013363	0.3191603	2.1228726
H	-4.3093825	-4.0036751	0.0046844

H	-4.5926788	-1.1497603	2.9105477
H	-6.1914774	-1.1483126	2.1529135
H	-5.6318655	-3.5892919	1.1061967
H	-6.0836730	0.0353644	-0.8559508
H	-6.8988347	-1.4779557	-0.4254313
H	-5.7851156	-1.4220438	-1.8058504
H	-1.9358653	-3.9548075	0.1456329
H	-4.1657077	-2.1786722	-3.1657076
H	-1.8682853	-0.5039943	-3.3178514
H	-0.3661216	-0.9399536	-2.4887901
H	-4.5306645	-3.3997373	-1.9383225
H	-1.0000463	-4.1831533	-1.3492533
H	-0.4746816	-3.0061295	-0.1312970
H	-3.2159173	-3.6663673	-3.0893132
H	-1.1501656	-2.1042547	-3.5728300

3a.xyz

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Energy = -2404.890649465

B	8.7626516	2.8018109	29.3838653
P	9.5396872	3.7220725	31.8441427
H	8.9943574	4.9546289	31.4128395
Si	11.6317169	5.9595221	31.7776691
Si	12.5772035	2.8422043	31.8000013
W	8.1718687	2.6456247	33.6692295
O	10.7660024	1.3781563	35.0771863
O	5.4328252	4.0176967	32.6962608
O	6.4624912	1.3301105	36.0202367
O	7.7527562	0.0899287	31.7600238
O	8.7220286	5.2933241	35.4043104
O	9.7216809	2.9771196	30.3810023
C	10.4506005	7.0850489	32.7213636
C	10.6806422	2.1706954	27.7034333
C	10.7969497	-0.1785477	26.7743547
C	11.0518275	1.3077799	26.4911940
C	11.3856613	6.1944112	29.9275140
C	11.2494625	4.1521377	32.2672162
C	11.8928762	1.0948082	31.6459732
C	13.3824313	6.4304579	32.2826645
C	13.4440846	3.2697274	30.1862557
C	13.8188067	2.8710928	33.2147687
C	4.8372921	3.3701768	29.0289460
C	4.9205708	4.6965498	28.2629654
C	6.1714601	2.6130985	28.9862143
C	6.0672927	5.5668212	28.7920905
C	6.4309386	3.5180681	32.9981505
C	7.0837466	1.8091165	35.1673137
C	7.3428848	3.4711030	29.5100643
C	7.4045294	4.8170561	28.7296801
C	7.8969038	0.9987096	32.4577995
C	8.5165979	4.3397871	34.7830213
C	8.9739321	0.4486745	28.4213071
C	9.3457873	-0.4179298	27.2104752
C	9.2156439	1.9586359	28.1327533
C	9.8498061	1.8222317	34.5275489
H	10.3950596	5.8573748	29.6019271
H	10.6631286	8.1334573	32.4781307
H	10.4489552	1.6207078	25.6264020
H	10.5698846	6.9625901	33.8041303
H	11.0316083	-0.7818536	25.8888885
H	10.8611529	3.2306955	27.4831861
H	11.4721494	-0.5118505	27.5760023
H	11.3347870	1.9075043	28.5436059
H	11.2592619	4.1346637	33.3679340
H	11.4699028	7.2585050	29.6755973
H	11.2734986	0.9814985	30.7530269
H	12.1313850	5.6487963	29.3420022
H	12.1035116	1.4677196	26.2218316
H	11.2980164	0.7902587	32.5112839
H	12.7370504	3.3473312	29.3558273
H	12.7376174	0.3984622	31.5662669
H	13.5548946	7.4881753	32.0473105
H	13.5280135	6.3035951	33.3617060
H	14.0063544	4.2071891	30.2455971
H	14.1500285	5.8461657	31.7658407
H	13.3443338	2.5749868	34.1578470
H	14.1573161	2.4716466	29.9440596
H	14.2610527	3.8628022	33.3557345
H	14.6343410	2.1649559	33.0162333
H	4.0396948	2.7417402	28.6139665
H	3.9698950	5.2382567	28.3363439
H	4.5723117	3.5746854	30.0747378
H	5.0895722	4.4895702	27.1961416
H	6.0941919	1.6903049	29.5735105
H	5.8616688	5.8443999	29.8353505
H	6.3817086	2.3114522	27.9506229
H	6.1369158	6.4988593	28.2176784
H	7.1266431	3.7252648	30.5585901
H	7.6590916	4.6133091	27.6798709
H	7.9289197	0.2737629	28.7002691
H	8.2062949	5.4510836	29.1308051
H	8.6714736	-0.1741747	26.3770481
H	8.5680408	2.2219708	27.2807345
H	9.1902760	-1.4774456	27.4495264
H	9.3979308	6.9005374	32.4792418
H	9.5844505	0.1478954	29.2838394

3bn^{-}.xyz

82

Energy = -3189.582826046

B	-1.1662299	-0.5273552	-0.2608546
P	1.5141753	0.1120724	0.2222473
H	1.0014579	0.1392146	1.5422611
Si	1.6492929	2.9712577	1.4522643

Si	1.5759256	2.4935632	-1.7718442
W	3.4627715	-1.5384761	0.0111235
O	5.2404877	0.6449224	-1.5287653
O	1.8537636	-3.7283675	1.7344151
O	5.8975035	-3.5880663	-0.1204761
O	2.5771936	-2.6420159	-2.8793708
O	4.6785695	-0.4592585	2.7784809
O	0.2077232	-0.0476369	-0.6720372
C	2.6013520	2.3207043	2.9468870
C	-0.1716142	3.0262773	1.8853202
C	2.0406272	1.8558218	-0.0330295
C	1.7198213	1.1639131	-3.0972057
C	2.2527954	4.7370530	1.1393203
C	-0.1439650	3.2475495	-1.8043563
C	2.8578416	3.8116187	-2.2260373
C	2.3786192	-2.9315405	1.0831791
C	5.0076341	-2.8396292	-0.0788772
C	2.8336370	-2.2418149	-1.8266310
C	4.2084288	-0.8322244	1.7863887
C	4.5835118	-0.1397841	-0.9806348
H	-0.5617739	2.0242702	2.0861228
H	2.4259482	2.9678776	3.8159608
H	3.6813760	2.2910916	2.7634869
H	3.1402235	1.8185573	-0.0570078
H	-0.3131325	3.6404335	2.7844034
H	0.9254609	0.4203294	-3.0068850
H	-0.7837355	3.4525624	1.0851278
H	2.6843634	0.6464652	-3.0517757
H	-0.9000470	2.5251532	-1.4835753
H	1.6457696	1.6344562	-4.0866836
H	2.1401039	5.3268876	2.0585117
H	3.3098528	4.7675895	0.8510502
H	-0.2184251	4.1289607	-1.1570219
H	1.6735785	5.2360170	0.3544828
H	3.8705121	3.3908389	-2.1955682
H	-0.3967893	3.5639381	-2.8244132
H	2.8351041	4.6838704	-1.5660702
H	2.6782459	4.1631007	-3.2505085
H	2.2864787	1.3084572	3.2230380
C	-2.6906289	1.0762691	0.3997982
C	-3.4607977	2.0048093	1.0825062
C	-2.9227114	0.7881994	-0.9591906
C	-4.4819288	2.6623061	0.3706054
H	-3.2764520	2.2151624	2.1317043
C	-3.9285582	1.4359152	-1.6635554
C	-4.7084905	2.3840462	-0.9764711
H	-5.0992880	3.3962255	0.8821453
H	-4.0997446	1.2127678	-2.7127963
H	-5.5025679	2.9033310	-1.5072535
O	-1.6654281	0.3277765	0.8805089
O	-2.0660529	-0.1513538	-1.4109631
N	-1.1965586	-2.0007533	0.1008340
Si	-1.2673258	-3.1459454	-1.2167664
Si	-1.7931932	-2.3875037	1.6953608
C	-0.0982813	-4.6151753	-0.9911457
C	-3.0234845	-3.8279332	-1.4283331
C	-0.8016556	-2.3633615	-2.8668641
C	-1.6752132	-4.2490239	2.0369279
C	-0.7944275	-1.5855336	3.0858892
C	-3.6214134	-1.9601314	1.9251449
H	-0.2266239	-5.3058702	-1.8357618
H	-3.0782611	-4.5096374	-2.2879028
H	0.9464505	-4.2878968	-0.9934824
H	-3.7166125	-2.9976526	-1.6101364
H	-3.3811870	-4.3741326	-0.5479908
H	-0.2691746	-5.1769182	-0.0692435
H	0.0534708	-1.6902302	-2.7736507
H	-1.6326463	-1.7834180	-3.2761869
H	-0.5319867	-3.1532261	-3.5799819
H	-4.2341565	-2.4941124	1.1883622
H	-0.6379663	-4.5958227	2.0738388
H	0.2613346	-1.8728657	3.0346990
H	-0.8611249	-0.4951318	3.0546296
H	-2.2163115	-4.8651265	1.3109570
H	-3.9653672	-2.2614171	2.9242954
H	-3.8167837	-0.8903252	1.8060696
H	-2.1231426	-4.4386467	3.0222839
H	-1.1801471	-1.9263187	4.0566730

3b.xyz

55

Energy = -2315.855674923

B	1.9738296	-1.4524350	-0.1060406
P	-0.4776740	-0.5911356	0.7035145
H	-0.2571849	-0.9675167	2.0493590
Si	-2.5499580	-2.6264352	1.6630621
Si	-2.0321834	-2.1349775	-1.5263526
W	-0.2942756	1.8807124	0.3556865
O	-2.8530770	1.8640417	-1.5851885
O	2.1697521	2.0351433	2.4218183
O	-0.1286777	5.0527551	0.0265352
O	1.7346695	1.3986765	-2.0956768
O	-2.3039531	2.1802243	2.8462979
O	0.6284293	-1.6146826	-0.0050360
C	-2.9356280	-1.5741132	3.1773138
C	-1.1590512	-3.8296597	2.0571141
C	-2.0150690	-1.4336044	0.2656326
C	-1.0042478	-1.1156178	-2.7306592
C	-4.1072932	-3.5685423	1.1885187
C	-1.4009437	-3.9048290	-1.5717950
C	-3.8250002	-2.0471062	-2.0914403
C	1.2981081	1.9536797	1.6700061
C	-0.1879279	3.9021903	0.1437564
C	1.0011614	1.5889838	-1.2237662

C	-1.5795445	2.0798647	1.9508201
C	-1.9197920	1.8564537	-0.9011279
H	-0.2286933	-3.3146475	2.3215600
H	-3.2781001	-2.2098295	4.0029411
H	-3.7296804	-0.8496324	2.9607103
H	-2.7693856	-0.6323608	0.2413646
H	-1.4466518	-4.4493636	2.9153203
H	0.0686640	-1.1895864	-2.5346362
H	-0.9445856	-4.4966319	1.2166265
H	-1.2822128	-0.0579722	-2.7367239
H	-0.3687965	-3.9626812	-1.2110942
H	-1.1834881	-1.5049894	-3.7414209
H	-4.4243690	-4.1886387	2.0364134
H	-4.9308078	-2.8859526	0.9500965
H	-2.0130492	-4.5884029	-0.9742948
H	-3.9555548	-4.2323116	0.3311576
H	-4.1821836	-1.0102602	-2.0851574
H	-1.4166372	-4.2665016	-2.6075646
H	-4.4954703	-2.6396828	-1.4615787
H	-3.9103049	-2.4222582	-3.1186837
H	-2.0633132	-1.0153191	3.5349504
C	4.0387065	-0.7346317	0.1722916
C	5.1896622	-0.0788615	0.5655125
C	4.0388706	-1.7141544	-0.8217485
C	6.3712278	-0.4552566	-0.0918947
H	5.1768448	0.6829138	1.3374847
C	5.1954530	-2.0950474	-1.4763021
C	6.3735892	-1.4386176	-1.0870131
H	7.3031070	0.0305682	0.1799411
H	5.1900995	-2.8564311	-2.2487923
H	7.3076907	-1.7017397	-1.5734927
O	2.7408682	-0.5628137	0.6465525
O	2.7422330	-2.1863450	-1.0094971

4b^{-}.xyz

42

Energy = -1909.241059344

P	-0.3741129	-0.5490639	0.2507517
H	-0.1010390	-0.7623146	1.6435672
Si	-2.2500574	-2.5551979	1.5967652
Si	-2.3243043	-2.0555574	-1.5873753
W	-0.4479743	2.0287062	-0.0212406
O	-3.3942048	1.8635682	-1.2856289
O	2.4625469	1.8401382	1.3318508
O	-0.3664341	5.2067526	-0.2147716
O	0.8907454	1.6650867	-2.9238115
O	-1.7938502	2.0805420	2.8928881
O	0.6286256	-1.3733007	-0.5570361
C	-2.4543482	-1.5642508	3.1925561
C	-0.7521659	-3.6916842	1.7446763
C	-2.0457680	-1.3536094	0.1520746
C	-1.6276249	-0.9537786	-2.9475215
C	-3.8003818	-3.6289695	1.4324191
C	-1.5428688	-3.7604379	-1.7731759
C	-4.1918156	-2.1720752	-1.8740942
C	1.4166716	1.9277625	0.8375500
C	-0.3991162	4.0402416	-0.1520129
C	0.4036403	1.8004234	-1.8814794
C	-1.3043285	2.0776904	1.8393921
C	-2.3221168	1.9340068	-0.8413822
H	0.1826598	-3.1359589	1.6143210
H	-2.6132345	-2.2379021	4.0445860
H	-3.3191981	-0.8924455	3.1284079
H	-2.8017878	-0.5656108	0.2895627
H	-0.7361747	-4.1740315	2.7303324
H	-0.5430538	-0.8624684	-2.8430800
H	-0.7743876	-4.4785409	0.9832246
H	-2.0623609	0.0507019	-2.9317294
H	-0.4760291	-3.6900078	-1.5356470
H	-1.8506099	-1.3986480	-3.9268087
H	-3.9068373	-4.2642802	2.3217785
H	-4.7062416	-3.0163580	1.3503542
H	-1.9968693	-4.5070704	-1.1117349
H	-3.7582070	-4.2867409	0.5572064
H	-4.6556687	-1.1820482	-1.7808904
H	-1.6491836	-4.1187780	-2.8052290
H	-4.6855310	-2.8422223	-1.1625781
H	-4.3999102	-2.5426903	-2.8863392
H	-1.5740050	-0.9496181	3.4074360

4.xyz

85

Energy = -3432.748722469

P	-0.0417646	1.3444988	15.8227540
H	-0.7067087	0.4159367	14.9566084
Si	-2.5650503	0.1118372	17.0562304
Si	-1.0011420	2.5138587	18.5076893
W	2.4523954	0.6715689	15.8588837
O	2.4142946	0.4407087	19.0638746
O	2.4553443	0.8397600	12.6502101
O	5.5128516	-0.2135243	15.8001636
O	3.1945629	3.7887836	16.0561065
O	1.3577643	-2.3430649	15.6617971
O	-0.4561620	2.7487020	15.3562834
C	-2.2237102	-1.6152713	16.3740528
C	-3.5601278	1.1200649	15.8050204
C	-0.9135466	0.9665867	17.4129045
C	0.5237758	3.6140245	18.3888463
C	-3.5997649	-0.1244622	18.6206050
C	-2.4901756	3.5694556	18.0373317
C	-1.1405356	1.9503731	20.3055230
C	2.4398343	0.7953617	13.8097265
C	4.3937799	0.1127106	15.8261183
C	2.9321234	2.6605155	15.9879614

C	1.7732308	-1.2628129	15.7335087
C	2.4261454	0.5325720	17.9070676
H	-2.9050487	1.7826283	15.2300995
H	-3.1675182	-2.1482258	16.2012401
H	-1.6288581	-2.2058500	17.0813369
H	-0.2948012	0.2394062	17.9594236
H	-4.0958937	0.4646035	15.1079112
H	0.6380349	4.0106823	17.3769592
H	-4.3014649	1.7531896	16.3054758
H	1.4425052	3.0826844	18.6566020
H	-2.4271738	3.8001187	16.9692423
H	0.4134657	4.4571934	19.0840768
H	-4.5152313	-0.6792701	18.3765231
H	-3.0559653	-0.6978165	19.3807025
H	-3.4453995	3.0663761	18.2223961
H	-3.8996989	0.8296648	19.0679137
H	-0.2642515	1.3534051	20.5872563
H	-2.4912393	4.5097485	18.6029953
H	-2.0328844	1.3433221	20.4886928
H	-1.1800556	2.8186716	20.9758067
H	-1.6762726	-1.5841802	15.4261456
K	-0.6610771	4.8586550	13.9773930
O	-1.5228887	3.2216408	11.7089770
O	-0.0688293	7.2353325	15.4559693
O	1.7784589	6.3924236	13.4471139
O	1.2160900	4.0057444	12.0462472
O	-3.4238272	4.2361956	13.5856796
O	-2.8089859	6.6157136	14.9642351
C	1.0962828	7.9865782	15.0954017
C	-0.4052850	2.3674589	11.4281467
C	-2.6422100	2.4655655	12.1858666
C	2.1861054	7.0372936	14.6605286
C	0.7468410	3.2167934	10.9495242
C	-1.1458550	8.0944117	15.8434285
C	-3.7816574	3.4133606	12.4728110
C	2.2983149	4.8627671	11.6794111
C	-2.3609202	7.2583155	16.1638503
C	2.8113180	5.5452862	12.9245455
C	-4.4221374	5.2120353	13.8862082
C	-4.0395114	5.9099933	15.1693189
H	0.8506174	8.6821185	14.2789855
H	1.4478958	8.5705735	15.9593820
H	-0.6752294	1.6438704	10.6440918
H	-0.1227580	1.8183374	12.3360720
H	-2.3584693	1.9199033	13.0962389
H	0.4207676	3.8706211	10.1264011
H	-2.9586526	1.7397339	11.4211614
H	2.3800375	6.2862242	15.4387970
H	-2.1232546	6.5026417	16.9268309
H	3.1099715	7.6108270	14.4900649
H	-1.3750971	8.7954385	15.0266705
H	-0.8610741	8.6761191	16.7333378
H	1.5537634	2.5652673	10.5856444
H	1.9584151	5.6054306	10.9415451
H	3.0962637	4.7981748	13.6762922
H	-3.9860940	4.0390925	11.5909337
H	-4.6872284	2.8347544	12.7103839
H	3.6975948	6.1469567	12.6718311
H	-3.1514614	7.9152926	16.5572878
H	3.1137773	4.2736022	11.2327075
H	-3.9196706	5.1754840	15.9775767
H	-4.5035779	5.9350466	13.0602807
H	-5.4004284	4.7262717	14.0231829
H	-4.8340431	6.6172007	15.4518437

5a^{-}.CO_2.xyz

79

Energy = -2593.082148949

B	-0.9830273	-0.6531665	-0.4910634
O	0.0519764	0.2183811	-0.2811044
P	1.5531822	-0.0191153	0.5262695
C	1.7170490	-1.6634953	3.6763149
O	0.8789653	-1.0687264	4.2356666
O	2.5662118	-2.2923246	3.1774003
Si	1.2641304	2.8292173	-0.9404709
Si	1.8583303	2.4455310	2.1915510
W	3.2695555	-1.4188649	-0.9402011
O	2.4373940	-4.2058310	0.4332704
O	0.7858125	-1.5987082	-2.9611393
O	5.3330809	-3.0892075	-2.6806368
O	5.2586954	-0.8884893	1.5232550
O	4.5094683	1.2241738	-2.2722456
C	-0.4131675	3.5261808	-0.4177547
C	0.1209165	2.1124965	2.8463286
C	2.6895731	-3.1782306	-0.0477390
C	1.7186849	-1.5470832	-2.2697178
C	1.0380154	1.9887101	-2.6144856
C	-0.8639334	-2.1360901	0.0600975
C	-2.2558279	0.0071535	-1.1905353
C	-1.6169330	-3.2558304	-0.6797820
C	2.0622932	1.7904369	0.4269654
C	-1.3837410	-4.6236956	-0.0215468
C	-2.5538822	-0.5359207	-2.6087283
C	-3.5323234	-0.0863256	-0.3206570
C	2.1906798	4.3058060	2.3520489
C	-1.2756030	-2.1265059	1.5576276
C	-3.7334571	0.2025518	-3.2568079
C	3.1519760	1.5985652	3.2777163
C	4.5769836	-2.4821143	-2.0232172
C	-4.7159819	0.6463974	-0.9680992
C	2.4214695	4.2969482	-1.2627547
C	-1.7721001	-4.6051573	1.4635196
C	4.5536574	-1.0967792	0.6223317
C	-1.0304381	-3.4908911	2.2145332

C	4.0187405	0.2806851	-1.8008707
C	-4.9915157	0.1182228	-2.3822526
H	-0.8664395	4.0724313	-1.2552930
H	-0.6199929	2.7546109	2.3581450
H	-0.1632165	1.0692390	2.6757307
H	-0.3256417	4.2228312	0.4238667
H	0.0793012	2.3040763	3.9260435
H	-1.0957922	2.7225326	-0.1267184
H	0.2933975	1.1921616	-2.5718785
H	0.2081897	-2.3951614	0.0442468
H	-1.3025863	-3.2905537	-1.7295869
H	-2.0299744	1.0787508	-1.3093348
H	0.6969375	2.7451941	-3.3349539
H	-0.3198763	-4.8837227	-0.1094060
H	-1.6622411	-0.4443521	-3.2389589
H	1.9706878	1.5654055	-2.9973749
H	-3.3396800	0.3285977	0.6772742
H	1.4627108	4.9119972	1.8015624
H	-3.4612285	1.2593564	-3.3947334
H	-1.9498396	-5.4021264	-0.5504157
H	-4.4819729	1.7196156	-1.0244895
H	-0.7178994	-1.3440729	2.0851144
H	2.1365890	4.5997272	3.4089771
H	0.0467876	-3.7061829	2.1986317
H	3.1610718	0.5163565	3.1168228
H	3.1410899	1.8148286	0.2166710
H	-2.7898214	-1.6065860	-2.5522744
H	2.9697115	1.7876872	4.3428519
H	2.0041082	4.9499938	-2.0408310
H	-3.8004169	-1.1423525	-0.1751359
H	-3.9372760	-0.2083756	-4.2546067
H	-2.3427170	-1.8754640	1.6398404
H	2.5863879	4.9049872	-0.3671656
H	-1.5632074	-5.5795363	1.9238976
H	3.1911679	4.5668168	1.9863653
H	-5.6137316	0.5466489	-0.3433983
H	3.3988038	3.9437787	-1.6143669
H	4.1552133	1.9707395	3.0338242
H	-2.8561346	-4.4362838	1.5504089
H	-5.8173666	0.6753784	-2.8434530
H	-1.3425454	-3.4676937	3.2672180
H	-5.3125134	-0.9321149	-2.3165328
H	-2.6949538	-3.0380682	-0.6796711

5a^{-}.HN(SiMe$_3$)$_2$.xyz

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Energy = -3278.580346908

B	0.3279494	-1.6790363	-0.9256588
O	-0.6515760	-1.3157422	-0.0439989
C	0.8535814	-0.7420200	-2.1060929
C	0.9308868	-3.1553970	-0.7733223
P	-1.4455013	0.2243029	0.1147318
C	0.2354614	-1.2192331	-3.4483575
C	2.3941936	-0.7535845	-2.2377362
H	0.5314519	0.2975143	-1.9410636
C	-0.0820421	-4.2077537	-0.2851024
C	2.1825399	-3.1872665	0.1429468
H	1.2791464	-3.4690579	-1.7739882
C	-2.2274950	-0.0012198	1.8251579
H	0.3904516	1.9140157	-0.1851131
W	-3.5215643	0.2650719	-1.5385276
C	0.7537319	-0.4280438	-4.6573977
H	-0.8541740	-1.1415541	-3.4052433
H	0.4689198	-2.2851569	-3.5916225
C	2.9015478	0.0523244	-3.4386710
H	2.7356164	-1.7935329	-2.3463948
H	2.8526186	-0.3653972	-1.3219691
C	0.5299304	-5.6124337	-0.2091227
H	-0.9602369	-4.2149642	-0.9391987
H	-0.4392816	-3.9172678	0.7090015
C	2.8007495	-4.5907478	0.2176114
H	2.9352425	-2.4726363	-0.2069376
H	1.8981385	-2.8712656	1.1545570
Si	-1.9039882	1.4513097	3.0011144
Si	-2.0847081	-1.7181232	2.6003843
H	-3.3140671	0.0597449	1.6660706
N	1.1642882	2.6012892	-0.2438040
C	-2.3485818	1.1676283	-2.9671631
C	-5.0331482	0.3586466	-2.8608058
C	-3.0107700	-1.6469112	-2.0766944
C	-3.9990956	2.0832862	-0.7208592
C	-4.8415738	-0.5489215	-0.1998653
C	2.2831662	-0.4588858	-4.7440977
H	0.3095256	-0.8288178	-5.5784427
H	0.4196660	0.6129038	-4.5730022
H	2.6358834	1.1072054	-3.3013595
H	3.9981817	0.0012418	-3.4881476
C	1.7736653	-5.6281397	0.6887561
H	0.8129784	-5.9402652	-1.2209350
H	-0.2136568	-6.3313365	0.1608915
H	3.1673408	-4.8737986	-0.7806054
H	3.6713472	-4.5852500	0.8879146
C	-1.5398799	3.0657818	2.1066756
C	-0.4900129	1.1545413	4.2242618
C	-3.4867705	1.7608476	3.9947039
C	-2.9324494	-3.0077545	1.5200250
C	-0.3165725	-2.2123525	3.0318222
C	-3.0456444	-1.7537794	4.2390762
Si	0.8503628	3.9583133	-1.2766657
Si	2.4724122	2.2338536	0.8278076
O	-1.7659282	1.7144912	-3.8097640
O	-5.9082324	0.4004659	-3.6326262
O	-2.7383752	-2.7483862	-2.3214600
O	-4.3149933	3.0840217	-0.2208669

O	-5.6452415	-0.9769627	0.5225232
H	2.6300641	0.1418289	-5.5953715
H	2.6189009	-1.4920032	-4.9227233
H	2.2232802	-6.6301973	0.7101579
H	1.4736259	-5.3900189	1.7198187
H	-1.4207369	3.8692090	2.8469473
H	-2.3642112	3.3440047	1.4429749
H	-0.6278831	3.0199574	1.5056119
H	-0.3334122	2.0596392	4.8258624
H	-0.7054492	0.3313994	4.9145235
H	0.4528327	0.9284698	3.7169851
H	-3.3600628	2.6299672	4.6535052
H	-4.3204559	1.9803315	3.3159779
H	-3.7772282	0.9077656	4.6154170
H	-2.5966825	-2.9575359	0.4832240
H	-4.0170698	-2.8537895	1.5375829
H	-2.7329447	-4.0194881	1.8966913
H	-0.2763310	-3.2733197	3.3104526
H	0.3555628	-2.0568527	2.1869091
H	0.0618513	-1.6311450	3.8794251
H	-4.0930119	-1.4616689	4.0994919
H	-2.6115559	-1.1027443	5.0061022
H	-3.0389104	-2.7787335	4.6348849
C	1.7363225	5.4878057	-0.6044525
C	1.4696799	3.6858024	-3.0381423
C	-0.9986974	4.2796089	-1.3330350
C	2.5320670	3.3962818	2.3185979
C	2.2233683	0.4794465	1.4588211
C	4.1305545	2.3830848	-0.0665732
H	2.8207137	5.3421541	-0.5273633
H	1.3616097	5.7573595	0.3894653
H	1.5688811	6.3441874	-1.2705470
H	1.2898119	4.5734096	-3.6592674
H	0.9521388	2.8424768	-3.5080691
H	2.5458059	3.4749369	-3.0559648
H	-1.5471703	3.3416681	-1.4656843
H	-1.2657956	4.9411014	-2.1661328
H	-1.3548581	4.7364770	-0.4041150
H	1.5938723	3.3541423	2.8834539
H	2.6904856	4.4371883	2.0141343
H	3.3475809	3.1196784	3.0002062
H	2.5490289	-0.2697972	0.7311975
H	1.1595588	0.2980318	1.6489160
H	2.7733095	0.2996347	2.3903726
H	4.1730258	1.7067192	-0.9277137
H	4.2971964	3.4021040	-0.4372972
H	4.9659226	2.1356164	0.6013924

5a⁻.xyz

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Energy = -2404.377605040

B	8.7734039	2.7536575	29.3995556
O	9.7089154	3.0402830	30.3588104
P	9.4298097	4.0514067	31.7325063
Si	11.7104801	5.9547950	31.7807462
Si	12.4506948	2.8235291	31.8580356
W	8.1220429	2.8028876	33.6874261
O	10.7644669	1.6855391	35.1240574
O	5.3060305	4.0435558	32.7519706
O	6.5019006	1.3371923	35.9901420
O	8.0210364	0.4758754	31.4826751
O	8.6701808	5.5385012	35.2713162
C	10.5887089	7.1861688	32.6701993
C	10.7416635	2.1371272	27.7671826
C	10.8417654	-0.1298974	26.6497636
C	11.1456574	1.3673160	26.5032772
C	11.5245418	6.2016587	29.9189471
C	11.2220257	4.1966612	32.2862611
C	11.7234178	1.0871593	31.7483187
C	13.4865362	6.3911524	32.2838530
C	13.3674058	3.1627102	30.2403554
C	13.7522393	2.7951283	33.2348779
C	4.8117002	3.1947155	28.9950855
C	4.8529744	4.5988723	28.3770420
C	6.1744218	2.4947292	28.8876265
C	5.9649428	5.4467334	29.0089181
C	6.3400778	3.5914132	33.0336981
C	7.0912659	1.8946686	35.1446232
C	7.3013512	3.3299800	29.5206619
C	7.3277000	4.7513350	28.8935957
C	8.0357603	1.2807786	32.3207584
C	8.4517421	4.5377122	34.7184756
C	8.9744021	0.4179524	28.2740437
C	9.3684253	-0.3609627	27.0113150
C	9.2580209	1.9350891	28.1227474
C	9.8294046	2.0762213	34.5523035
H	10.5282052	5.8810573	29.5943402
H	10.8388514	8.2164084	32.3848143
H	10.5879917	1.7654797	25.6421798
H	10.6891054	7.1016339	33.7591007
H	11.0983930	-0.6665330	25.7269544
H	10.9597184	3.2060534	27.6463416
H	11.4743334	-0.5456580	27.4479479
H	11.3517719	1.7892843	28.6093378
H	11.1895142	4.1979489	33.3857863
H	11.6418561	7.2629085	29.6643940
H	10.9621248	1.0253769	30.9678679
H	12.2668623	5.6323931	29.3506053
H	12.2124563	1.5173412	26.2891532
H	11.2701906	0.7682949	32.6908829
H	12.6749361	3.2919912	29.4049675
H	12.5297919	0.3803779	31.5089323
H	13.7021705	7.4381478	32.0326592
H	13.6270010	6.2742187	33.3656288

H	13.9925516	4.0603371	30.3068609
H	14.2340709	5.7677299	31.7810312
H	13.2920016	2.5542552	34.2003872
H	14.0260324	2.3162833	30.0052870
H	14.2593433	3.7614888	33.3345486
H	14.5169263	2.0341984	33.0295041
H	4.0342606	2.5899506	28.5091495
H	3.8810540	5.0956187	28.4947161
H	4.5374207	3.2793651	30.0555516
H	5.0383162	4.5115284	27.2956545
H	6.1230800	1.5109162	29.3698618
H	5.7395204	5.6045761	30.0725896
H	6.4035796	2.3146503	27.8264604
H	6.0032566	6.4370984	28.5353333
H	7.0611881	3.4672957	30.5863743
H	7.6055910	4.6740673	27.8309057
H	7.9181204	0.2463894	28.5071734
H	8.0982215	5.3504411	29.3951986
H	8.7353783	-0.0299727	26.1745223
H	8.6547673	2.2774855	27.2624875
H	9.1769863	-1.4331610	27.1527466
H	9.5396052	7.0003236	32.4153711
H	9.5473276	0.0348258	29.1293209

5.xyz

119

Energy = -3927.851705331

B	-1.0590998	-1.5052161	1.4114696
O	0.1852101	-1.4428801	0.8554911
P	1.5642541	-0.4353598	0.7668589
Si	2.4988079	-3.4935393	1.1780166
Si	2.9144448	-1.9070493	-1.5619287
W	2.5627700	0.7164519	2.9396871
O	0.2090807	2.9002854	2.8464182
O	1.0505442	-0.8947783	5.2779106
O	3.9398407	2.5028209	5.1776404
O	4.5072810	2.0206669	0.7518885
O	4.9109825	-1.4471723	3.2965012
C	1.3299342	-4.6196120	0.2105601
C	1.2079594	-2.0800197	-2.3517105
C	1.0554152	2.1011643	2.8351508
C	1.5445396	-0.3165711	4.4052954
C	1.8298244	-3.3749325	2.9340373
C	-1.4756147	-0.6197118	2.6619127
C	-2.0400988	-2.4368586	0.5535360
C	-1.9684360	-1.4322618	3.8829817
C	2.7613312	-1.8205530	0.3143002
C	-2.3828426	-0.5200928	5.0455024
C	-3.2754586	-3.0752617	1.2117807
C	-2.4811753	-1.6143466	-0.6874894
C	3.9963898	-3.3329766	-2.1775315
C	-2.5510524	0.4139366	2.2522399
C	-4.0695983	-3.9302053	0.2125844
C	3.7516547	-0.3276380	-2.1694127
C	3.4331858	1.8411077	4.3648738
C	-3.2743193	-2.4635961	-1.6877943
C	4.1741621	-4.3633857	1.2811969
C	-3.4638588	0.4763749	4.6089782
C	3.7627484	1.5784010	1.5311903
C	-2.9804906	1.3135722	3.4183405
C	4.0501883	-0.6848718	3.1509817
C	-4.4906598	-3.1138644	-1.0162513
H	0.3375150	-4.1706228	0.1110304
H	0.7047392	-2.9916460	-2.0162264
H	0.5737484	-1.2354710	-2.0608262
H	1.2161620	-5.5708134	0.7460409
H	1.2746020	-2.1169613	-3.4460250
H	1.6993779	-4.8520258	-0.7941021
H	0.9212115	-2.7718628	2.9935730
H	-0.5926484	-0.0487191	2.9842012
H	-1.1839525	-2.1215701	4.2139283
H	-1.4220189	-3.2585076	0.1579027
H	1.5886914	-4.3864689	3.2869024
H	-1.5052490	0.0324786	5.4040726
H	-2.9740337	-3.6937617	2.0651373
H	2.5616268	-2.9531050	3.6279352
H	-1.6002766	-1.1818321	-1.1744341
H	3.5923015	-4.3185136	-1.9250173
H	-3.4413867	-4.7715624	-0.1140523
H	-2.7427372	-1.1258536	5.8865723
H	-2.6172544	-3.2482809	-2.0889726
H	-2.1606647	1.0277281	1.4296442
H	4.0878985	-3.2830683	-3.2706780
H	-2.1268724	1.9278096	3.7317576
H	3.1698503	0.5600256	-1.9068298
H	3.7414430	-1.4751775	0.6748978
H	-3.9344369	-2.2906088	1.6105969
H	3.8909610	-0.3322080	-3.2581659
H	4.0669195	-5.3261000	1.7977415
H	-3.1089512	-0.7724976	-0.3623801
H	-4.9529004	-4.3631417	0.6988773
H	-3.4351199	-0.1100264	1.8612584
H	4.6028682	-4.5640436	0.2939894
H	-3.7416190	1.1314850	5.4439059
H	5.0082882	-3.2706393	-1.7603168
H	-3.5957091	-1.8487042	-2.5398433
H	4.8942838	-3.7627516	1.8475307
H	4.7417594	-0.2244977	-1.7085856
H	-4.3711562	-0.0749280	4.3199727
H	-5.0296445	-3.7480243	-1.7313179
H	-3.7720765	2.0029399	3.0925105
H	-5.1899985	-2.3249628	-0.7008101
H	-2.8298682	-2.0466436	3.5945246
K	0.1242703	2.0884767	-1.4193170

O	-0.2314291	1.2492393	-4.2785540
O	-0.1369746	4.4152298	0.2248199
O	2.1203172	4.2792710	-1.3860739
O	2.1752442	2.4301343	-3.4813223
O	-2.5101327	1.3016218	-2.6386172
O	-2.5362890	3.3739497	-0.7330758
C	0.9471854	5.3301586	0.3939536
C	1.0234786	0.8330531	-4.8254015
C	-1.2332356	0.2301651	-4.3568576
C	2.2266231	4.6362739	-0.0022983
C	1.9539889	2.0220087	-4.8291599
C	-1.3855708	5.0063941	0.5799585
C	-2.5581592	0.8545926	-3.9943632
C	3.1271509	3.4931350	-3.3899589
C	-2.4492366	3.9365465	0.5827082
C	3.3562764	3.8062878	-1.9316940
C	-3.7097241	1.9922179	-2.2835141
C	-3.6173702	2.4460373	-0.8477027
H	0.7842111	6.2190740	-0.2344639
H	1.0116669	5.6427226	1.4470912
H	0.8841424	0.4781022	-5.8586627
H	1.4471259	0.0169978	-4.2271119
H	-0.9905221	-0.6013233	-3.6815716
H	1.5158176	2.8510275	-5.4060794
H	-1.2925671	-0.1623158	-5.3840403
H	2.3885468	3.7422627	0.6130156
H	-2.2028981	3.1576514	1.3143988
H	3.0748769	5.3202785	0.1506889
H	-1.6363865	5.8032791	-0.1372611
H	-1.3229044	5.4427730	1.5883729
H	2.9075997	1.7320110	-5.2982250
H	2.7465545	4.3792248	-3.9205530
H	3.6997675	2.9151405	-1.3930205
H	-2.7624414	1.7087819	-4.6578861
H	-3.3611703	0.1114385	-4.1189167
H	4.1303680	4.5844432	-1.8430268
H	-3.4142349	4.3873486	0.8624686
H	4.0784097	3.1845906	-3.8502535
H	-3.4578132	1.5887690	-0.1801824
H	-3.8462662	2.8587128	-2.9484557
H	-4.5772183	1.3226186	-2.3954864
H	-4.5645938	2.9327053	-0.5654957

6a⁻.xyz

79

Energy = -2593.090468579

B	-0.6766886	0.4459406	1.0731321
O	0.2660292	-0.3954031	0.1798658
P	1.5152435	0.4133921	-0.4010912
C	0.7935231	2.1064320	0.0286317
O	-0.3042607	1.9153982	0.7245815
O	1.2854310	3.1911231	-0.2478255
Si	0.8736678	-1.6577526	-2.5623497
Si	0.6973101	1.4834124	-3.3237617
W	3.8563200	0.1618714	0.5827163
O	3.0761809	2.1469097	2.9987156
O	2.8815056	-2.4527325	2.1812969
O	6.7822855	-0.0687606	1.8222983
O	4.7436737	2.7122150	-1.1655248
O	4.8259977	-1.6764745	-1.8603396
C	-0.9940314	-1.7193207	-2.7867608
C	-1.0187655	2.0121397	-2.7635566
C	3.3194930	1.4235370	2.1315296
C	3.2245921	-1.5030501	1.6177343
C	1.3570319	-2.9000704	-1.2310991
C	-0.2342982	0.2160909	2.6217872
C	-2.1882899	0.1987450	0.5347974
C	-0.3772531	-1.2235519	3.1481138
C	1.4686464	0.1310274	-2.2210943
C	0.2864461	-1.3888720	4.5230749
C	-2.6987973	-1.2493331	0.6548749
C	-3.2550725	1.1595135	1.0932300
C	0.5283547	0.8682684	-5.1098139
C	-0.8456188	1.1944610	3.6424401
C	-4.0358375	-1.4413380	-0.0761353
C	1.8706705	2.9505190	-3.4069567
C	5.7118343	0.0166346	1.3722863
C	-4.5996869	0.9908497	0.3696237
C	1.7366617	-2.2512801	-4.1386717
C	-0.2997579	-0.3973828	5.5384514
C	4.4039628	1.8093299	-0.5272678
C	-0.1973381	1.0471189	5.0274199
C	4.4536507	-1.0238517	-0.9738743
C	-5.0954400	-0.4605574	0.4468586
H	-1.4905019	-1.3206301	-1.8975751
H	-1.7143173	1.1669873	-2.7445577
H	-1.0236040	2.4725117	-1.7726033
H	-1.3250144	-2.7568547	-2.9217625
H	-1.4079837	2.7509890	-3.4767339
H	-1.3341098	-1.1447072	-3.6549482
H	0.8671437	-2.6879093	-0.2785741
H	0.8528519	0.4239692	2.6196209
H	0.0525855	-1.9335232	2.4322259
H	-2.1296261	0.4136583	-0.5483673
H	1.0525082	-3.9008505	-1.5670481
H	1.3656497	-1.2070960	4.4229339
H	-1.9493032	-1.9509624	0.2683741
H	2.4383701	-2.9262582	-1.0651664
H	-2.9073062	2.1957729	1.0100124
H	-0.1618874	0.0257793	-5.2207558
H	-3.8847178	-1.2668671	-1.1518874
H	0.1707758	-2.4187765	4.8894185
H	-4.4712431	1.2702037	-0.6869039
H	-0.7402624	2.2248294	3.2834648

H	0.1432242	1.6947189	-5.7223183
H	0.8627114	1.3285543	4.9538885
H	2.0183066	3.3963794	-2.4196463
H	2.5289419	0.1196241	-2.5169480
H	-2.8418524	-1.5012487	1.7146259
H	1.4699498	3.7183987	-4.0818320
H	1.4711097	-3.2998737	-4.3270959
H	-3.4036299	0.9616813	2.1646810
H	-4.3936796	-2.4753337	0.0308775
H	-1.9244456	0.9998833	3.7359184
H	1.4694315	-1.6736255	-5.0275446
H	0.2052355	-0.4977364	6.5093661
H	1.4961607	0.5722530	-5.5306851
H	-5.3561987	1.6694310	0.7890127
H	2.8256608	-2.2055961	-4.0167483
H	2.8488438	2.6416483	-3.7963643
H	-1.3601501	-0.6432140	5.7051274
H	-6.0352681	-0.5763990	-0.1109283
H	-0.6611556	1.7356673	5.7483630
H	-5.3174991	-0.7049102	1.4969340
H	-1.4430805	-1.4757660	3.2448123

6.xyz

122

Energy = -4116.632969451

B	-1.2048067	1.9017239	16.7900389
O	0.0523916	1.1380924	17.2421695
P	1.4275780	1.9323422	17.0677684
C	0.6849633	3.1897178	15.8877117
O	-0.6143744	3.0232380	15.8444511
O	1.2779135	4.0954000	15.2997719
Si	2.2799027	-0.9968388	16.9155131
Si	2.6901366	0.8666943	14.3066335
W	2.5305092	3.2360227	18.9579052
O	0.4465903	5.6616408	18.5995886
O	0.6587190	1.6781772	21.0613512
O	3.9335600	4.9264436	21.2651880
O	4.3642992	4.6378779	16.7212214
O	4.8302727	1.0220319	19.3040117
C	0.9980441	-1.9292206	15.9042085
C	1.0020701	0.8250806	13.4759436
C	1.1611967	4.7602567	18.7236091
C	1.3239321	2.2483759	20.3083490
C	1.7389303	-1.0081181	18.7196289
C	-1.8242086	2.6811647	18.0729207
C	-2.0698261	0.9170341	15.8413400
C	-2.4278487	1.7729355	19.1594042
C	2.5542197	0.7737972	16.2088964
C	-2.8119577	2.5672785	20.4161514
C	-2.5707665	-0.3785760	16.5074713
C	-3.2425198	1.5807744	15.0943743
C	3.6972196	-0.5811563	13.6311880
C	-2.8152455	3.8100375	17.7394085
C	-3.1562426	-1.3474580	15.4697636
C	3.6334275	2.4209216	13.8247322
C	3.4187495	4.3092162	20.4242015
C	-3.8429413	0.6363541	14.0427612
C	3.9471145	-1.8787101	16.8637697
C	-3.7884536	3.7014180	20.0741978
C	3.6933041	4.1341688	17.5193229
C	-3.2130237	4.6161090	18.9837814
C	3.9803804	1.8005659	19.1774469
C	-4.2945597	-0.6871905	14.6773412
H	0.0569358	-1.3722778	15.8825142
H	0.4374463	-0.0683432	13.7585777
H	0.3871682	1.6952561	13.7202575
H	0.8025983	-2.9059430	16.3641318
H	1.1422594	0.8001890	12.3879056
H	1.3184238	-2.1056962	14.8722507
H	0.7557988	-0.5514031	18.8545216
H	-0.9535359	3.1745922	18.5453385
H	-1.7222647	0.9736356	19.4159372
H	-1.3571691	0.5966077	15.0598945
H	1.6859094	-2.0536377	19.0516221
H	-1.9031500	2.9966765	20.8603572
H	-1.7580777	-0.8613016	17.0637395
H	2.4526784	-0.4949360	19.3714839
H	-2.9180634	2.5124383	14.6185282
H	3.2363351	-1.5581232	13.8057351
H	-2.3593136	-1.6484965	14.7733206
H	-3.2537235	1.9043100	21.1723110
H	-3.0797857	0.4263288	13.2779066
H	-2.3693065	4.4714194	16.9871216
H	3.7966209	-0.4507099	12.5453170
H	-2.3225397	5.1282983	19.3746213
H	3.1021404	3.3231599	14.1353443
H	3.5545838	1.0530514	16.5727270
H	-3.3512722	-0.1376368	17.2419859
H	3.7710196	2.4549456	12.7361832
H	3.8463880	-2.8704749	17.3230210
H	-4.0289585	1.8501371	15.8146107
H	-3.5189406	-2.2642228	15.9540552
H	-3.7225683	3.3829139	17.2889339
H	4.3358928	-2.0167271	15.8514325
H	-4.0307346	4.2835618	20.9729096
H	4.7083620	-0.5998619	14.0531708
H	-4.6879354	1.1144063	13.5272990
H	4.6938416	-1.3217363	17.4424239
H	4.6276536	2.4257205	14.2881836
H	-4.7319421	3.2645260	19.7134208
H	-4.6733779	-1.3723348	13.9074782
H	-3.9428710	5.3964615	18.7245796
H	-5.1316866	-0.4841907	15.3618895
H	-3.3311994	1.2851513	18.7664437

K	-0.6404648	5.4643086	13.8325149
O	-0.8297659	4.2309612	11.1846576
O	-0.7278866	7.5316563	15.7309640
O	1.6278004	7.2705837	14.1304512
O	1.6274231	5.2547982	12.1181415
O	-3.1104087	4.4723686	12.8395182
O	-3.1756261	6.6726558	14.6177249
C	0.4277680	8.3622295	15.8886500
C	0.4344382	3.7074383	10.7580438
C	-1.8369978	3.2137201	11.2511494
C	1.6592887	7.5645084	15.5338109
C	1.4516383	4.8237092	10.7691183
C	-1.9426541	8.2599128	15.9256981
C	-3.1641403	3.8718494	11.5424323
C	2.6799762	6.2140897	12.2585012
C	-3.0995959	7.2906572	15.9098682
C	2.8138556	6.5759145	13.7180053
C	-4.3247232	5.1600654	13.1571741
C	-4.2316315	5.7042493	14.5620254
H	0.3460353	9.2429467	15.2341594
H	0.5005377	8.7038788	16.9319658
H	0.3466990	3.2980266	9.7404597
H	0.7533949	2.9037952	11.4354186
H	-1.5852481	2.4840336	12.0348248
H	1.1140725	5.6628514	10.1418191
H	-1.9031791	2.6837520	10.2893732
H	1.6955588	6.6283644	16.1062761
H	-2.9600100	6.5228788	16.6821904
H	2.5527379	8.1615035	15.7723030
H	-2.0567144	9.0156077	15.1337094
H	-1.9244937	8.7738149	16.8986547
H	2.4027820	4.4454921	10.3638589
H	2.4566941	7.1088916	11.6585768
H	2.9435818	5.6731083	14.3263366
H	-3.3790159	4.6400223	10.7848857
H	-3.9610531	3.1138931	11.5119117
H	3.6916618	7.2271704	13.8497523
H	-4.0325786	7.8352805	16.1196499
H	3.6284430	5.7824104	11.9044733
H	-4.0326481	4.8940929	15.2768162
H	-4.4875919	5.9763371	12.4377792
H	-5.1762826	4.4655240	13.0986756
H	-5.1899628	6.1772585	14.8246324

CO_2.xyz

3

Energy = -188.6977308775

C	0.0000000	0.0000002	0.0000310
O	0.0000138	0.0000361	1.1686463
O	-0.0000130	-0.0000349	-1.1686849

K^+.OEt_2.xyz

58

Energy = -1757.270171439

K	-0.6510173	5.7161228	13.4515663
O	-0.5714934	4.0832918	11.1301889
O	-0.7688393	7.6896633	15.4607107
O	1.6543920	7.2590920	14.0466806
O	1.8451062	5.0375692	12.2929690
O	-3.0313373	4.4942505	12.5101018
O	-3.1686114	6.7315897	14.2609305
C	0.3240160	8.6159264	15.5036387
C	0.6879900	3.4194750	10.9594228
C	-1.6716225	3.1675992	11.0505060
C	1.6170704	7.8511860	15.3523097
C	1.7905124	4.4509171	10.9859179
C	-2.0336189	8.3459327	15.6179504
C	-2.9609273	3.9410158	11.1887076
C	2.8746094	6.0301542	12.3942177
C	-3.1312323	7.3100979	15.5726685
C	2.8897630	6.5742107	13.8027288
C	-4.2331882	5.2507218	12.7103058
C	-4.2410009	5.7915507	14.1199164
H	0.2202252	9.3548054	14.6954793
H	0.3287881	9.1475660	16.4664130
H	0.7081025	2.8959854	9.9925744
H	0.8321313	2.6798679	11.7607696
H	-1.5880894	2.4117388	11.8454863
H	1.6017363	5.2310165	10.2340456
H	-1.6619561	2.6534157	10.0784975
H	1.6929347	7.0680545	16.1214594
H	-2.9503252	6.5257769	16.3225367
H	2.4627246	8.5432882	15.4743712
H	-2.1735907	9.0857077	14.8160806
H	-2.0679738	8.8670084	16.5858528
H	2.7485554	3.9638083	10.7527585
H	2.6857219	6.8391200	11.6734856
H	3.0162615	5.7577357	14.5294662
H	-3.0029368	4.7487151	10.4435043
H	-3.8105437	3.2636043	11.0196286
H	3.7334334	7.2708674	13.9120458
H	-4.0929628	7.7939806	15.7964185
H	3.8533049	5.5818476	12.1691814
H	-4.1214927	4.9736969	14.8460050
H	-4.2796995	6.0754475	11.9842630
H	-5.1118575	4.6056902	12.5647229
H	-5.2034893	6.2878224	14.3111381
O	-0.4938127	3.7037713	15.2559883
C	0.7235143	3.4142397	15.9748162
C	1.6933986	2.5849057	15.1419506
H	0.4834097	2.9126966	16.9205259
H	1.1571036	4.3894778	16.2187730
H	2.6120415	2.4027041	15.7110605
H	1.2614500	1.6130810	14.8812784

H	1.9516178	3.1137100	14.2193124
C	-1.4922605	2.6656194	15.3512671
C	-2.2910751	2.7550806	16.6455615
H	-1.0131979	1.6826720	15.2511293
H	-2.1440490	2.8153326	14.4854072
H	-3.0623115	1.9768946	16.6610495
H	-1.6532077	2.6140164	17.5237616
H	-2.7802722	3.7309928	16.7272804

K⁺.xyz K(18-crown-6)⁺

43

Energy = -1523.452450113

K	-0.6336195	5.8464783	13.1970043
O	-0.4568844	4.2424696	10.8963107
O	-0.8067888	7.4422547	15.5054729
O	1.6113455	7.3203995	14.0377083
O	1.8888392	5.2821023	12.0924341
O	-2.8767436	4.3620528	12.3646529
O	-3.1568269	6.4067206	14.3087041
C	0.2211785	8.4354933	15.6351792
C	0.8443511	3.6964579	10.6345308
C	-1.4857364	3.2505332	10.7649634
C	1.5602460	7.7828603	15.3951714
C	1.8650452	4.8027615	10.7399318
C	-2.1079809	7.9864524	15.7706097
C	-2.8242174	3.9043123	11.0050843
C	2.8762440	6.3072626	12.2761220
C	-3.1279293	6.8796070	15.6639433
C	2.8790120	6.7242600	13.7261976
C	-4.1436601	4.9612098	12.6754367
C	-4.1409114	5.3776643	14.1256449
H	0.0515077	9.2443639	14.9096118
H	0.2029905	8.8628280	16.6479198
H	0.8749512	3.2709871	9.6213228
H	1.0656574	2.8978786	11.3575996
H	-1.3173315	2.4406630	11.4897240
H	1.6116863	5.6267784	10.0569355
H	-1.4675681	2.8241511	9.7518190
H	1.7050220	6.9367940	16.0827959
H	-2.8707368	6.0523553	16.3414318
H	2.3583437	8.5183153	15.5707518
H	-2.3311026	8.7867961	15.0500049
H	-2.1375381	8.4094000	16.7849068
H	2.8541679	4.4100736	10.4642226
H	2.6465793	7.1662054	11.6288202
H	3.0516454	5.8543518	14.3765722
H	-2.9666245	4.7532186	10.3205855
H	-3.6233238	3.1709196	10.8258467
H	3.6861385	7.4520754	13.8920989
H	-4.1164690	7.2694846	15.9454748
H	3.8703815	5.9218757	12.0081833
H	-3.9070723	4.5195299	14.7723952
H	-4.3135596	5.8316065	12.0251022
H	-4.9521784	4.2352794	12.5084370
H	-5.1360218	5.7593451	14.3950759

na.xyz $N(SiMe_3)_2BCy_2$

62

Energy = -1369.353965186

B	0.0006021	0.0004472	-0.4362287
C	0.9537348	-2.4745517	-0.4067178
C	0.6450648	-4.0173575	-2.3877186
C	1.5862088	-3.5835912	-1.2563612
C	-0.2250226	2.8128576	-3.2488813
C	-0.6425682	4.0159288	-2.3935608
C	0.3974350	1.7024047	-2.3914978
C	-1.5790142	3.5868604	-1.2565374
C	-0.5545748	1.2527686	-1.2521788
C	-0.9451968	2.4778787	-0.4078445
C	-0.4004608	-1.7064429	-2.3853020
C	0.2205483	-2.8170570	-3.2435134
C	0.5561011	-1.2520784	-1.2515934
H	2.5256131	-3.2107699	-1.6909396
H	1.1232677	-4.7810879	-3.0136893
H	1.6348954	-2.1785795	0.3984329
H	-0.2515901	-4.4797387	-1.9493894
H	0.0561050	-2.8694798	0.0885427
H	1.8454591	-4.4455167	-0.6281039
H	0.4804577	3.1283246	-4.0283327
H	-1.1221811	4.7793852	-3.0187867
H	-1.1105379	2.4092144	-3.7613653
H	0.2573079	4.4772491	-1.9607457
H	0.6710634	0.8516770	-3.0248540
H	-2.5216147	3.2156212	-1.6855228
H	1.3321671	2.0758620	-1.9476357
H	-1.8328174	4.4507167	-0.6287122
H	-1.4721157	0.8893530	-1.7544735
H	-0.0441061	2.8716014	0.0821491
H	-0.6795492	-0.8576890	-3.0189633
H	-1.6230421	2.1850914	0.4012738
H	1.1025707	-2.4122824	-3.7610950
H	1.4702142	-0.8874070	-1.7591242
H	-0.4879439	-3.1357837	-4.0188919
H	-1.3319172	-2.0814861	-1.9359535
N	-0.0005469	0.0004512	1.0356380
Si	1.4839010	0.4294347	1.8586611
Si	-1.4859756	-0.4289090	1.8566760
C	1.9142073	-0.8071102	3.2127069
C	2.8799553	0.4998050	0.5931766
C	1.3898063	2.1322999	2.6632822
C	-1.9133849	0.8020563	3.2167139
C	-2.8826433	-0.4896036	0.5914205
C	-1.3956397	-2.1358121	2.6531392
H	1.9636284	-1.8319500	2.8291197

H	2.6573644	1.2057696	-0.2165340
H	1.1799133	-0.7863501	4.0267741
H	3.0959712	-0.4734871	0.1409275
H	3.7955915	0.8499897	1.0859494
H	2.8907066	-0.5574919	3.6472299
H	1.2200006	2.9189568	1.9199884
H	2.3361873	2.3521975	3.1749006
H	0.5868827	2.1954791	3.4046821
H	-0.5911393	-2.2050094	3.3923378
H	-1.9601655	1.8289074	2.8382038
H	-3.0964966	0.4865598	0.1443442
H	-2.6620471	-1.1918587	-0.2220298
H	-1.1794675	0.7754182	4.0309263
H	-2.3415250	-2.3550959	3.1659285
H	-1.2300959	-2.9195453	1.9057914
H	-2.8906391	0.5527121	3.6496741
H	-3.7989129	-0.8401567	1.0827589

nb.xyz N(SiMe$_3$)$_2$Bcat

40

Energy = -1280.342597606

B	-0.4341387	0.0487003	-0.0933526
C	-2.5843769	-0.5255580	0.0639561
C	-3.7935157	-1.1570969	0.2952324
C	-2.5097439	0.7403867	-0.5216666
C	-4.9496854	-0.4574646	-0.0877452
H	-3.8439775	-2.1405788	0.7508402
C	-3.6408257	1.4402453	-0.9026227
C	-4.8751221	0.8106011	-0.6726379
H	-5.9212776	-0.9138719	0.0756033
H	-3.5753301	2.4233734	-1.3569804
H	-5.7897133	1.3222469	-0.9567085
O	-1.3094185	-0.9751634	0.3470524
O	-1.1853602	1.1164828	-0.6379408
N	0.9751837	-0.0118463	-0.0009598
Si	1.9330014	1.4755534	0.1762696
Si	1.7268752	-1.6268921	0.0568082
C	2.8464328	1.8723614	-1.4168247
C	0.8278915	2.9273093	0.6240417
C	3.1362217	1.2566566	1.6085858
C	3.4624114	-1.5586647	-0.6683959
C	1.7745687	-2.2441953	1.8296846
C	0.7549891	-2.8214487	-1.0214680
H	3.3817452	2.8253190	-1.3194430
H	1.4684522	3.7746861	0.9012285
H	3.5776434	1.1030948	-1.6839758
H	0.1862343	2.6999209	1.4832561
H	0.1855452	3.2385559	-0.2037823
H	2.1378434	1.9688105	-2.2481675
H	3.8317555	0.4212661	1.4872229
H	2.5865137	1.1034845	2.5450153
H	3.7343468	2.1701274	1.7198672
H	0.6204066	-2.4176387	-2.0323491
H	4.1417473	-0.8640339	-0.1666611
H	2.3744324	-1.5876608	2.4696283
H	0.7597837	-2.2840793	2.2425773
H	3.4308943	-1.2966962	-1.7320412
H	1.3157494	-3.7606192	-1.1115572
H	-0.2316470	-3.0506113	-0.6105908
H	3.9016106	-2.5615802	-0.5887819
H	2.2027927	-3.2528008	1.8836494

nH.xyz HN(SiMe$_3$)$_2$

28

Energy = -874.2186972187

H	-0.0003360	-0.0000148	-1.8254237
N	-0.0000580	-0.0000037	-0.8088961
Si	-0.0051606	1.5883450	-0.0931230
Si	0.0051470	-1.5883444	-0.0930947
C	-1.7288869	2.0864963	0.4854082
C	1.1517993	1.6203801	1.3927315
C	0.5814015	2.8036805	-1.4048713
C	-1.1518124	-1.6205020	1.3927637
C	-0.5813248	-2.8036995	-1.4048644
C	1.7289067	-2.0863546	0.4854456
H	-1.7288249	3.0945689	0.9197104
H	1.1501194	2.6121168	1.8622087
H	-2.4392365	2.0788001	-0.3503019
H	2.1811259	1.3858740	1.0975131
H	0.8501302	0.8962359	2.1592715
H	-2.1050603	1.3937699	1.2476774
H	-0.0695185	2.7768285	-2.2880652
H	1.6025916	2.5731534	-1.7311257
H	0.5739761	3.8311780	-1.0209794
H	2.4392560	-2.0786599	-0.3502603
H	-2.1811025	-1.3857748	1.0975937
H	-1.6025339	-2.5732560	-1.7311174
H	0.0695884	-2.7767837	-2.2880603
H	-0.8500325	-0.8965534	2.1594457
H	2.1050543	-1.3935607	1.2476649
H	1.7289015	-3.0944030	0.9198049
H	-1.1502985	-2.6123182	1.8620719
H	-0.5738116	-3.8311986	-1.0209792

K$^+$.n$^-$.xyz K(18-crown-6)$^+$ N(SiMe$_3$)$_2^-$

70

Energy = -2397.182058602

K	-0.3426665	4.8062462	13.9504184
O	-0.2150452	3.9126039	11.0760373
O	-0.7120647	7.1456367	15.5421731
O	1.6896334	7.0352768	14.1146316
O	2.1683579	4.9198265	12.2643958
O	-2.6331206	3.9499696	12.4736989
O	-3.0560412	5.9300232	14.4745359

C	0.2218730	8.2247314	15.5761074
C	1.0820115	3.4038552	10.7468796
C	-1.2519429	2.9651537	10.7978462
C	1.6115828	7.6599080	15.4010424
C	2.0851622	4.5213696	10.8917066
C	-2.0371339	7.5515128	15.8980515
C	-2.5852229	3.6133983	11.0872573
C	3.0375184	6.0480093	12.4116084
C	-2.9384229	6.3417083	15.8416674
C	3.0012146	6.5309789	13.8402764
C	-3.9330956	4.3768449	12.8920264
C	-3.8651636	4.7534995	14.3523506
H	-0.0065119	8.9455935	14.7770364
H	0.1662886	8.7447785	16.5445774
H	1.0938816	3.0499942	9.7047095
H	1.3380567	2.5596389	11.4033327
H	-1.1205544	2.0684517	11.4199563
H	1.7767659	5.3813783	10.2785139
H	-1.2150807	2.6665704	9.7390299
H	1.8278603	6.9263614	16.1906852
H	-2.5196762	5.5211429	16.4405071
H	2.3473943	8.4756837	15.4686793
H	-2.3914055	8.3273142	15.2029985
H	-2.0398078	7.9632906	16.9185092
H	3.0690190	4.1751845	10.5392197
H	2.7110257	6.8538813	11.7373692
H	3.2488189	5.7157213	14.5356230
H	-2.7173526	4.5193079	10.4766805
H	-3.3886859	2.9028198	10.8399061
H	3.7460020	7.3317676	13.9646586
H	-3.9291730	6.6071787	16.2422066
H	4.0684862	5.7667831	12.1469620
H	-3.4240055	3.9387285	14.9434287
H	-4.2563801	5.2388571	12.2896604
H	-4.6565445	3.5589080	12.7558988
H	-4.8822429	4.9549642	14.7230534
N	-0.6753724	2.9431742	16.0892285
Si	0.2751020	3.4124556	17.3916569
Si	-0.8796960	1.4200540	15.4114642
C	0.4830165	2.1660343	18.8214001
C	2.0698480	3.8403060	16.8829318
C	-0.3758831	4.9806808	18.2526191
C	-0.7137423	-0.0899578	16.5659424
C	-2.5914544	1.1968578	14.6088444
C	0.3703612	1.0654656	14.0064442
H	1.0161321	2.6323730	19.6620542
H	2.6742063	4.2166801	17.7203050
H	-0.4898442	1.8195819	19.1927263
H	2.0884444	4.6061976	16.0963826
H	2.5721874	2.9525891	16.4758783
H	1.0519138	1.2794081	18.5177626
H	-1.3979303	4.8261727	18.6236033
H	-0.3928900	5.8384411	17.5713726
H	0.2544001	5.2450457	19.1131640
H	0.3232718	1.8374970	13.2275824
H	-1.3805151	-0.0070682	17.4335217
H	-3.3898900	1.3699115	15.3425152
H	-2.7403825	1.8972358	13.7799557
H	0.3077724	-0.2061132	16.9475426
H	1.3965701	1.0680108	14.3972577
H	0.1966460	0.0973464	13.5160712
H	-0.9749597	-1.0126994	16.0286051
H	-2.7130427	0.1779014	14.2157668

n$^-$.xyz $N(SiMe_3)_2^-$

27

Energy = -873.6285672814

N	0.0000000	0.0000000	0.6524479
Si	0.0000000	1.5802211	0.1825607
Si	0.0000000	-1.5802211	0.1825607
C	1.5124072	2.1232723	-0.8649156
C	-1.5124072	2.1232723	-0.8649156
C	0.0000000	2.7707415	1.6794266
C	1.5124072	-2.1232723	-0.8649156
C	0.0000000	-2.7707415	1.6794266
C	-1.5124072	-2.1232723	-0.8649156
H	1.4938978	3.1940029	-1.1193758
H	-1.4938978	3.1940029	-1.1193758
H	2.4463643	1.9209301	-0.3234779
H	-2.4463643	1.9209301	-0.3234779
H	-1.5530472	1.5555046	-1.8047007
H	1.5530472	1.5555046	-1.8047007
H	0.8842280	2.5961308	2.3072070
H	-0.8842280	2.5961308	2.3072070
H	0.0000000	3.8296968	1.3809532
H	-2.4463643	-1.9209301	-0.3234779
H	2.4463643	-1.9209301	-0.3234779
H	0.8842280	-2.5961308	2.3072070
H	-0.8842280	-2.5961308	2.3072070
H	1.5530472	-1.5555046	-1.8047007
H	-1.5530472	-1.5555046	-1.8047007
H	-1.4938978	-3.1940029	-1.1193758
H	1.4938978	-3.1940029	-1.1193758
H	0.0000000	-3.8296968	1.3809532

OEt_2.xyz

15

Energy = -233.7997570882

O	0.0000683	-0.0000492	0.8569313
C	0.0614778	1.2022747	0.0695328
C	-0.0614555	-1.2023371	0.0694855
C	1.4799058	1.5166269	-0.3974631
C	-1.4799176	-1.5165751	-0.3974856
H	0.3097086	-1.9972117	0.7240451

H	-0.3097294	1.9971091	0.7241199
H	0.6227167	-1.1273290	-0.7876486
H	-0.6227056	1.1272448	-0.7875867
H	1.4892172	2.4575236	-0.9602382
H	-1.4893373	-2.4575089	-0.9601950
H	1.8698159	0.7295584	-1.0515653
H	-1.8697477	-0.7295115	-1.0516400
H	2.1499032	1.6180408	0.4621623
H	-2.1499204	-1.6178555	0.4621513

TS34^{-}.xyz

82

Energy = -3189.595228720

B	-3.1201168	-0.8038178	-0.1717795
P	0.3206883	0.6840322	0.2492370
H	0.0430754	0.5696631	1.6484110
Si	0.0254851	3.3913869	1.7040872
Si	0.0201187	3.1974811	-1.5195091
W	2.5356910	-0.6189502	-0.1504768
O	3.8024235	1.8414763	-1.7758955
O	1.3063434	-2.8697028	1.7847015
O	5.1845472	-2.3481883	-0.5355006
O	1.4226766	-1.7361698	-2.9537261
O	3.7856739	0.7220792	2.4818067
O	-0.9650553	0.3416308	-0.5122847
C	1.1061444	2.8750686	3.1655807
C	-1.7645323	2.9656885	2.0889236
C	0.6274507	2.5162523	0.1441932
C	0.2430747	1.9839908	-2.9456396
C	0.1776132	5.2738935	1.5630362
C	-1.7895623	3.7048543	-1.4466394
C	1.0770113	4.7173568	-1.9238856
C	1.7222702	-2.0757717	1.0463693
C	4.2194254	-1.7117609	-0.4014445
C	1.7845192	-1.3534677	-1.9218703
C	3.3113194	0.2349565	1.5389391
C	3.3290957	0.9451011	-1.2057051
H	-1.9281903	1.8834008	2.0920552
H	0.7858852	3.3963003	4.0769452
H	2.1600896	3.1192906	2.9900584
H	1.7194037	2.6506794	0.1299992
H	-2.0432138	3.3591529	3.0751721
H	-0.4124492	1.1203376	-2.8074912
H	-2.4455688	3.3937565	1.3478988
H	1.2737733	1.6219643	-3.0215061
H	-2.4075831	2.8599923	-1.1309005
H	-0.0070843	2.4816884	-3.8923557
H	-0.1034857	5.7434899	2.5151899
H	1.2060343	5.5775084	1.3327896
H	-1.9618533	4.5337097	-0.7506740
H	-0.4757048	5.6830111	0.7844192
H	2.1387386	4.4457458	-1.9774540
H	-2.1384858	4.0242385	-2.4369083
H	0.9703772	5.5113832	-1.1770906
H	0.7904239	5.1325643	-2.8991990
H	1.0436684	1.7983511	3.3544292
C	-4.2558411	1.0855267	0.1792333
C	-4.8852608	2.2005843	0.7034935
C	-4.2490724	0.8209270	-1.1950706
C	-5.5101590	3.0660667	-0.2105049
H	-4.8840762	2.4011330	1.7695548
C	-4.8630750	1.6651974	-2.1037348
C	-5.4978178	2.8050278	-1.5832387
H	-6.0064782	3.9582122	0.1605613
H	-4.8441272	1.4575989	-3.1688995
H	-5.9831733	3.4982946	-2.2642010
O	-3.5826644	0.0893580	0.8416577
O	-3.5881164	-0.3534500	-1.4368629
N	-2.6327092	-2.1126148	0.1074960
Si	-2.1706654	-3.1679534	-1.2364310
Si	-2.7996519	-2.6374381	1.7890189
C	-0.5602754	-4.0850191	-0.9193449
C	-3.5513446	-4.4291566	-1.5059318
C	-1.9149882	-2.1925909	-2.8189872
C	-2.1262370	-4.3756503	2.0600685
C	-1.8862800	-1.4956978	2.9677683
C	-4.6341645	-2.6805182	2.2267297
H	-0.3272272	-4.6744345	-1.8161463
H	-3.3207323	-5.0882136	-2.3530054
H	0.2610509	-3.3791825	-0.7680756
H	-4.4949152	-3.9148941	-1.7252471
H	-3.7144444	-5.0619350	-0.6254619
H	-0.5864053	-4.7672075	-0.0673544
H	-1.3580502	-1.2747219	-2.6087311
H	-2.8601621	-1.9163815	-3.2937970
H	-1.3308208	-2.8039969	-3.5187660
H	-5.1697749	-3.3788358	1.5714816
H	-1.0341614	-4.4065718	2.0058506
H	-0.8164958	-1.4814304	2.7429715
H	-2.2609146	-0.4712215	2.9012263
H	-2.5313432	-5.1190163	1.3654709
H	-4.7844971	-3.0079540	3.2636416
H	-5.0882684	-1.6908660	2.1113004
H	-2.4163188	-4.6812290	3.0745685
H	-2.0118981	-1.8469902	4.0002077

TS45^{-}.xyz

104

Energy = -3278.583735284

B	1.6056664	-1.7123633	-0.4652578
O	0.6224825	-1.3153728	0.4199106
C	2.1414107	-0.8021139	-1.6498883
C	2.1405113	-3.2089245	-0.3134208
P	-0.2563110	0.1238530	0.5410297

C	1.4682038	-1.2651761	-2.9719174
C	3.6763104	-0.8973573	-1.8178186
H	1.8861170	0.2540843	-1.4788699
C	1.0870417	-4.2243599	0.1686686
C	3.4020398	-3.3140537	0.5849970
H	2.4651249	-3.5243231	-1.3210981
C	-0.9394630	-0.0042201	2.2690889
H	0.8860815	1.2347900	0.4589868
W	-2.2746874	0.1768447	-1.0938567
C	1.9912956	-0.5053411	-4.1984124
H	0.3832646	-1.1415839	-2.9034851
H	1.6523482	-2.3408798	-3.1126199
C	4.1903561	-0.1214944	-3.0352931
H	3.9605433	-1.9536917	-1.9325336
H	4.1737805	-0.5319882	-0.9136073
C	1.6373530	-5.6559201	0.2023204
H	0.1995058	-4.1789857	-0.4718061
H	0.7590014	-3.9430824	1.1753870
C	3.9570932	-4.7448909	0.6165398
H	4.1787490	-2.6236638	0.2401277
H	3.1459545	-3.0076612	1.6070198
Si	-0.6510225	1.4541261	3.4684995
Si	-0.8427257	-1.7338369	3.0599145
H	-2.0247641	0.0737601	2.1026239
N	2.0366448	2.2491472	0.2947701
C	-1.1569261	1.0520656	-2.5906216
C	-3.8176954	0.2570852	-2.3946169
C	-1.8098563	-1.7396599	-1.6793923
C	-2.8054096	1.9904288	-0.2924188
C	-3.5916279	-0.6339792	0.2442264
C	3.5152453	-0.6086388	-4.3220799
H	1.5055041	-0.8897706	-5.1052224
H	1.7104944	0.5510371	-4.1101658
H	3.9777877	0.9454541	-2.8970513
H	5.2809075	-0.2269355	-3.1120452
C	2.8924876	-5.7475103	1.0794677
H	1.8900790	-5.9710032	-0.8212528
H	0.8679490	-6.3491603	0.5678463
H	4.2961535	-5.0190947	-0.3934828
H	4.8359688	-4.7924237	1.2732845
C	-0.3289406	3.0657309	2.5692753
C	0.7360425	1.1431573	4.7103939
C	-2.2649813	1.7042793	4.4242353
C	-1.7064035	-3.0029359	1.9658733
C	0.9012354	-2.2745010	3.5093783
C	-1.8325690	-1.7390219	4.6748261
Si	1.8272516	3.6074751	-0.7033576
Si	3.4018568	1.9426371	1.2508284
O	-0.6371592	1.5550340	-3.4952239
O	-4.7024483	0.3007804	-3.1474166
O	-1.5880053	-2.8399402	-1.9624419
O	-3.1851615	2.9704436	0.1990517
O	-4.4139122	-1.0564122	0.9486872
H	3.8671289	-0.0284436	-5.1849823
H	3.7962552	-1.6571203	-4.5040272
H	3.2972099	-6.7679193	1.0680299
H	2.6188079	-5.5230508	2.1209511
H	-0.1373768	3.8597183	3.3034416
H	-1.2044916	3.3590459	1.9800433
H	0.5317021	2.9985586	1.8934768
H	0.8805537	2.0434913	5.3213729
H	0.4997910	0.3160125	5.3891457
H	1.6882735	0.9195751	4.2210470
H	-2.1833488	2.6032170	5.0491721
H	-3.0980779	1.8631116	3.7276356
H	-2.5257853	0.8653486	5.0753013
H	-1.3953526	-2.9353975	0.9221127
H	-2.7913629	-2.8596378	2.0136851
H	-1.4886219	-4.0184108	2.3204732
H	0.8734936	-3.2933502	3.9172923
H	1.5632036	-2.2699207	2.6427399
H	1.3367097	-1.6206186	4.2720202
H	-2.8690887	-1.4180271	4.5203984
H	-1.3922197	-1.1089963	5.4548204
H	-1.8588070	-2.7683950	5.0576561
C	2.6234670	5.2021739	-0.0256809
C	2.5499961	3.3989783	-2.4484840
C	0.0008606	4.0424579	-0.9426858
C	3.5651751	3.0756573	2.7749529
C	3.3440969	0.1743805	1.9230277
C	5.0660558	2.1280812	0.3429061
H	3.7125857	5.1105294	0.0735179
H	2.2201768	5.4484406	0.9645869
H	2.4216921	6.0522525	-0.6928092
H	2.3927903	4.2997942	-3.0581466
H	2.0826567	2.5560456	-2.9700589
H	3.6292547	3.2053145	-2.4048507
H	-0.5889573	3.1656214	-1.2250428
H	-0.1208598	4.7938677	-1.7341522
H	-0.4360261	4.4461756	-0.0228983
H	2.6472793	3.0761090	3.3734552
H	3.7603100	4.1118544	2.4728002
H	4.3911836	2.7544811	3.4252424
H	3.4967205	-0.5598516	1.1249987
H	2.3750783	-0.0494941	2.3797687
H	4.1191589	0.0005142	2.6806455
H	5.1012856	1.5075886	-0.5597792
H	5.2304029	3.1682381	0.0326957
H	5.9081042	1.8374491	0.9869583

TS56$^-$.xyz

79

Energy = -2593.079584961

B	-2.4121253	0.2130371	-0.1031821

O	-1.3964710	-0.7085930	-0.0468171	H	-1.3232127	-2.3273631	-2.8174692
P	0.2061412	-0.6637558	-0.6460743	H	-1.7750839	-4.8028272	0.2553406
C	0.4023542	0.1395724	-3.3460895	H	-1.1214849	-3.9649526	-3.4637555
O	-0.5061648	-0.3943116	-3.8855688	H	-2.5691547	-3.2236431	0.4052104
O	1.3597992	0.8135318	-3.1812465	H	-1.3038145	-1.1024638	2.4372182
Si	-0.2689181	-3.1182239	1.3714455	H	-1.1072292	1.7516629	-0.9408480
Si	0.5614862	-3.5067541	-1.6976788	H	-2.3930467	2.9348795	0.8672638
W	1.8193005	0.9579130	0.6694636	H	-3.6360973	-1.3616770	0.7814075
O	1.2406243	3.4498172	-1.2817799	H	-1.1194276	-2.4485967	3.5775784
O	-0.7265146	1.6459074	2.4958152	H	-1.3599117	4.2796653	-0.9369353
O	3.8092052	2.9109329	2.1892581	H	-3.1052731	0.2500247	2.6063857
O	4.0167991	-0.1398737	-1.4020062	H	0.2735838	-1.4388722	3.1673544
O	2.8876693	-1.3195571	2.6588132	H	-4.8956499	-0.6049688	-1.2455893
C	-1.9088658	-3.9349797	0.9105097	H	0.1040824	-5.7887033	-0.7029043
C	-1.1141466	-3.3650311	-2.5443113	H	-5.0381690	-1.2804457	2.8841689
C	1.3957070	2.5224387	-0.6016276	H	-2.8918983	5.0029719	-0.4406498
C	0.2128916	1.4143406	1.8534434	H	-6.1259446	-1.7960647	0.5488311
C	-0.6315110	-1.8979566	2.7613633	H	-2.3683580	0.6393562	-2.8106755
C	-2.1956698	1.5986332	-0.8464970	H	0.9035206	-5.8972931	-2.2785414
C	-3.7606226	-0.2837106	0.5909337	H	-1.3044687	2.8644256	-3.1702592
C	-2.7754294	2.8513117	-0.1557522	H	1.9702614	-1.8972503	-3.0236427
C	0.6359108	-2.4214382	-0.1455299	H	1.6963334	-2.3938800	0.1454875
C	-2.4477782	4.1308259	-0.9388715	H	-4.1349966	1.4559697	1.8485077
C	-3.9919886	0.3748340	1.9756181	H	1.8528548	-3.4672268	-3.8409764
C	-5.0339621	-0.1230684	-0.2694142	H	0.3686214	-4.8856449	3.0132428
C	0.8797547	-5.3395557	-1.3326346	H	-5.2110013	0.9434904	-0.4674463
C	-2.7529114	1.5241160	-2.2946107	H	-5.3747204	0.2756555	3.6495475
C	-5.2215756	-0.2154915	2.6793995	H	-3.8459226	1.4245400	-2.2541918
C	1.9508911	-2.9790693	-2.8631988	H	1.0837217	-5.2528858	1.4339617
C	3.0820943	2.1951082	1.6161711	H	-2.6468996	4.9465349	-2.9446232
C	-6.2674757	-0.7117120	0.4299837	H	1.8460316	-5.4887998	-0.8361173
C	0.8522137	-4.4426543	2.1324463	H	-7.1611962	-0.5722490	-0.1927266
C	-2.9394053	4.0453301	-2.3902805	H	1.7997092	-3.9989605	2.4614314
C	3.2299654	0.2796487	-0.6588389	H	2.9238731	-3.2623018	-2.4415871
C	-2.3977944	2.7897722	-3.0868268	H	-4.0393163	4.0094752	-2.3960569
C	2.4491671	-0.5161767	1.9411075	H	-7.3425342	-0.5359123	2.3129535
C	-6.4795049	-0.0788368	1.8116146	H	-2.7949551	2.7206814	-4.1082691
H	-2.4149051	-4.2802405	1.8214994	H	-6.7126854	0.9888700	1.6847555
H	-1.9210315	-3.7246822	-1.8981014	H	-3.8675003	2.7482091	-0.0778016