Selective Phosphanyl Complex Trapping using TEMPO. Synthesis and reactivity of *P*-Functional *P*-Nitroxyl Phosphane Complexes

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Supporting Information

A. General information

All manipulations involving air- and moisture sensitive compounds were carried out under an atmosphere of purified argon by using standard Schlenk-line techniques or in a glove-box. Solvents were dried with appropriate drying agents and degassed before use. The ^{1}H, $^{13}C\{^{1}H\}$, and $^{31}P\{^{1}H\}$ NMR spectroscopic data were recorded on a Bruker DMX 300 spectrometer. Mass spectra were recorded on a MAT 95 XL Thermo Finnigan spectrometer (selected data given). Infrared spectra were recorded on a Thermo Nicolet 380 FT-IR spectrometer (selected data given).

B. Experimental procedures and analytical data

One-electron oxidation with $[Ph_3C]BF_4$ in the presence of TEMPO.

Complex $(CO)_5W\{(Me_3Si)_2HCP(F)TEMPO\}$ (3a). To a stirred solution of phosphane complex **1** (534.2 mg, 1 mmol) and 12-crown-4 (0.175 mL, 1.12 mmol) in 18 mL of THF at –78 °C was slowly added solution of *n*-BuLi (1.6 M, 0.7 mL, 1.12 mmol). After 15 min the mixture was cooled down up to –90 °C and a mixture of triphenylcarbenium tetrafluoroborate (380 mg, 1.15 mmol) and TEMPO (781 mg, 5 mmol) was added under argon atmosphere as a solid. Stirred reaction mixture was slowly warmed up to –30 °C in a cooling bath (ca. 2.5 h). Volatiles were removed under reduced pressure (0.02 mbar). Crude product was extracted with *n*-pentane (ca. –20 °C) and subjected to column chromatography (Al_2O_3, –20 °C, petrol ether). After evaporation of the solvent, the residue was kept at 22 °C/1.1x10^{-5} mbar for 1 h to afford the product as a white solid. Yield: 475.1 mg (0.689 mmol, 68.9 %), m.p. 68 °C (dec.). ^{1}H NMR (300.13 MHz, $CDCl_3$, 25°C): δ = 0.30 (s, 9H, $Si(CH_3)_3$), 0.32 (s, 9H, $Si(CH_3)_3$), 1.20 (s, 6H, $2CH_3$), 1.33 (s, 3H, CH_3), 1.37 (s, 3H, CH_3), 1.35–1.71 (m, 7H, $3CH_2$, PCH). $^{13}C\{^{1}H\}$ NMR (125.77 MHz, $CDCl_3$, 25°C): δ = 3.4 (pt, $^{3}J_{C,P}$ = 2.6 Hz, $^{4}J_{C,F}$ = 2.6 Hz, $Si(CH_3)_3$), 3.4 (dd, $^{3}J_{C,P}$ = 1.8 Hz, $^{4}J_{C,F}$ = 1.8 Hz, $Si(CH_3)_3$), 16.5 (s, 4-CH_2), 21.2 (s, CH_3), 21.2 (s, CH_3), 22.2 (s, CH_3), 33.6 (d, $^{4}J_{C,P}$ = 14.0 Hz, CH_3), 34.8 (s, CH_3), 36.6 (dd, $^{1}J_{C,P}$ = 19.6 Hz, $^{2}J_{C,F}$ = 8.2 Hz, PCH), 40.3 (s, 3-CH_2), 41.4 (s, 3-CH_2), 61.9 (s, $\underline{C}(CH_3)_2$), 62.5 (dd, $^{3}J_{C,P}$ = 5.2 Hz, $^{4}J_{C,F}$ = 5.2 Hz, $\underline{C}(CH_3)_2$, $^{1}J_{C,W}$ = 127.0), 197.5 (dd, $^{2}J_{C,P}$ = 8.2 Hz, $^{3}J_{C,F}$ = 3.0 Hz, *cis*-CO), 198.9 (dd, $^{2}J_{C,P}$ = 36.4 Hz, $^{4}J_{C,F}$ = 2.9 Hz, *trans*-CO). $^{31}P\{^{1}H\}$ NMR (121.51 MHz, $CDCl_3$; 25 °C): δ = 216.6 (d_{sat}, $^{1}J_{P,W}$ = 338.6 Hz, $^{1}J_{P,F}$ = 997.4 Hz). $^{19}F\{^{1}H\}$ NMR (282.37 MHz, $CDCl_3$; 25 °C): δ = –22.7 (d_{sat}, $^{1}J_{F,W}$ = 20.0 Hz, $^{1}J_{F,P}$ = 997.4 Hz). MS (EI, 70 eV, ^{184}W): 550.1 $[M - TEMP + H]^{\cdot+}$, 622.1 $[M - TEMP + SiMe_3]^{\cdot+}$. IR ($\nu$(CO), neat): 2072 (m), 1985 (m), 1916 (vs), 1900 (vs) cm^{-1}. Elemental analysis (%): $C_{21}H_{37}FNO_6PSi_2W$ (689.50): C 36.58, H 5.41. Found: C 36.99, H 5.44.

One-electron oxidation with $[TEMPO]BF_4$.

General procedure. To a stirred solution of corresponding phosphane complex $(CO)_5W\{(Me_3Si)_2HCP(H)F\}$ (534.2 mg, 1 mmol) or $(CO)_5W\{(Me_3Si)_2HCPH_2\}$ (434 mg, 1 mmol) and 12-crown-4 (0.175 mL, 1.12 mmol) in 18 mL of THF at –78 °C was slowly added solution of *n*-BuLi (1.6 M, 0.7 mL, 1.12 mmol). After 30 min the mixture was cooled down up to –90 °C and $[TEMPO]BF_4$ (292 mg, 1.2 mmol) was added under argon atmosphere as a solid. Stirred reaction mixture was warmed up to –30 °C in a cooling bath (ca. 1 h). Volatiles were removed under reduced pressure (0.02 mbar). Crude product was extracted with *n*-pentane (ca. –20 °C) and washed with the same solvent at –45 °C. The residue was kept at 22 °C/0.011 mbar for 2 h to afford the product as a white solid.

Complex $(CO)_5W\{(Me_3Si)_2HCP(F)TEMPO\}$ (3a) Yield: 518 mg (0.75 mmol, 75 %). Analytical data are identical to those, shown above.

Complex $(CO)_5W\{(Me_3Si)_2HCP(H)TEMPO\}$ (3b) Yield: 537 mg (0.80 mmol, 80 %), m.p. 128 °C (dec.). ^{1}H NMR (300.13 MHz, $CDCl_3$, 25°C): δ = 0.23 (s_{Sat}, $^{2}J_{H,Si}$ = 119.4 Hz, 9H, $Si(CH_3)_3$), 0.25 (s_{Sat}, $^{2}J_{H,Si}$ = 119.4 Hz, 9H, $Si(CH_3)_3$), 0.9–1.5 (m, 6H, $3CH_2$), 1.05 (s, 3H, CH_3), 1.09 (s, 3H, CH_3), 1.26 (s, 6H, $2CH_3$), 1.53 (dd, $^{2}J_{H,P}$ = 4.9 Hz, $^{3}J_{H,H}$ = 3.3 Hz, 1H, PCH). $^{13}C\{^{1}H\}$ NMR (125.77 MHz, $CDCl_3$, 25°C): δ = 1.6 (d_{Sat}, $^{3}J_{C,P}$ = 3.0 Hz, $^{1}J_{C,Si}$ = 52.4 Hz, $Si(CH_3)_3$), 2.7 (d_{Sat}, $^{3}J_{C,P}$ = 2.6 Hz, $^{1}J_{C,Si}$ = 52.4 Hz, $Si(CH_3)_3$), 16.7 (s, 4-CH_2), 21.0 (s, CH_3), 22.1 (s, CH_3), 23.1 (d_{Sat}, $^{1}J_{C,P}$ = 1.6 Hz, $^{1}J_{C,Si}$ = 35.6 Hz, PCH), 34.6 (s, CH_3), 35.4 (s, CH_3), 40.6 (s, 3-

CH_2), 41.4 (s, 3-CH_2), 62.4 (d, $^3J_{C,P}$ = 10.4 Hz, 2C(CH_3)$_2$), 198.1 (d_{Sat}, $^2J_{C,P}$ = 6.8 Hz, $^1J_{C,W}$ = 126.3 Hz, *cis*-CO), 199.0 (d, $^2J_{C,P}$ = 26.7 Hz, *trans*-CO). $^{31}P\{^1H\}$ NMR (121.51 MHz, $CDCl_3$; 25 °C): δ = 111.3 (s_{sat}, $^1J_{P,W}$ = 272.1 Hz). MS (EI, 70 eV, ^{184}W), m/z (%): 671.2 (5) $[M]^+$. IR (ν(CO), neat): 2075 (m), 1930 (vs), 1904 (vs) cm^{-1}. Elemental analysis (%): $C_{21}H_{38}NO_6PSi_2W$ (671.51): C 37.56, H 5.70, N 2.09. Found: C 37.95, H 5.32, N 2.10.

Thermolysis of 3a.

Complex $(CO)_5W\{(Me_3Si)_2HCP(F)SiMe_3\}$ (6). Phosphane complex **3a** (150 mg, 0.217 mmol) was dissolved in 2 mL toluene and heated for 1 hour. Solvent was removed under reduced pressure (0.02 mbar). Crude product was extracted with *n*-pentane (ca. –20 °C) and was purified using column chromatography [–20 °C, Al_2O_3, *n*-pentane with TMSCl (ca. 2 %)]. After evaporation of volatiles, the residue was washed with *n*-pentane at –45 °C to afford the product as a white solid. Yield: 20 mg (0.032 mmol, 15 %), m.p. 63 °C (dec.). ^1H NMR (300.13 MHz, $CDCl_3$, 25°C): δ = 0.15 (d, $^4J_{C,P}$ =1.6 Hz, 9H, Si(CH_3)$_3$), 0.21 (s, 9H, Si(CH_3)$_3$), 0.22 (s, 9H, Si(CH_3)$_3$), 1.50 (pt, 1H, CHPF). $^{13}C\{^1H\}$ NMR (125.77 MHz, $CDCl_3$, 25°C):δ = 1.4 (s, Si(CH_3)$_3$); 1.9 (d, $^3J_{C,P}$ = 2.6 Hz , Si(CH_3)$_3$), 2.3 (pt, $^3J_{C,P}$ = 2.5 Hz, $^4J_{C,F}$ = 2.5 Hz, Si(CH_3)$_3$), 40.6 (dd, $^1J_{C,P}$ = 10.5 Hz, $^2J_{C,F}$ = 4.8 Hz, PCH), 197.1 (dd_{Sat}, $^1J_{C,W}$ = 126.5, $^2J_{C,P}$ = 9.3 Hz, $^3J_{C,F}$ = 2.3 Hz, *cis*-CO), 198.9 (dd, $^2J_{C,P}$ = 33.0 Hz, $^4J_{C,F}$ = 3.3 Hz, *trans*-CO). $^{31}P\{^1H\}$ NMR (121.51 MHz, $CDCl_3$; 25 °C): δ = 191.3 (d_{sat}, $^1J_{P,W}$ = 342.1, $^1J_{P,F}$ = 989.3). $^{19}F\{^1H\}$ NMR (282.37 MHz, $CDCl_3$; 25 °C): δ = –29.4 (d, $^1J_{P,F}$ = 989.4). MS (EI, 70 eV, ^{184}W): 622.2 $[M]^+$. [IR (ν(CO), neat): 2074 (m), 1965 (m), 1914 (vs) cm^{-1}. Elemental analysis (%): $C_{15}H_{28}FO_6PSi_3W$ (622.45): C 28.94, H 4.53. Found: C 29.02, H 4.77.

Complex [TEMP-2H]$(CO)_5W\{(Me_3Si)_2HCP(F)O\}$ (5). Complex **5** was formed selectively from **3a** (250 mg, 0.362 mmol) in 18 mL of toluene, after heating at 40 °C for 80 min. $^{31}P\{^1H\}$ NMR (121.51 MHz, toluene (reaction solution); 25 °C): δ = 157.9 ppm ($d_{Sat,}$ $^1J_{P,W}$ = 309.8 Hz, $^1J_{P,F}$ = 952.9 Hz); the signal was the only one observed in the whole +1340 ÷ –710 ppm region of the spectrum. After evaporation of volatiles and extraction with *n*-pentane, obtained solution in ^{31}P NMR spectrum displayed the only signal of complex **6**. Single crystals of **5** were obtained during extraction with *n*-pentane at ca. 24 °C on the walls of a Schlenck-tube under intensive argon flow.

Crystallographic data.

Complex 3a ($C_{21}H_{37}FNO_6PSi_2W$): M = 689.52, triclinic, P -1, a = 13.1797(3) Å, b = 14.2791(3) Å, c = 15.1502(3) Å, V = 2825.91(10) Å^3, Z = 4; $d_{calc.}$ = 1.621 Mg/m^3, μ = 4.269 mm^{-1}, T = 123(2) K. A total 34076 reflections were measured on a Nonius KappaCCD diffractometer using monochromated Mo Kα radiation (λ = 0.71073 Å), 12234 reflections were unique (R_{int} = 0.0404). A semiempirical absorption correction from equivalents was applied (min/max transmission 0.2800/0.4822). The structure was solved with Patterson methods and refined with full-matrix least-squares against F^2 of all reflections. Non-hydrogen atoms were refined anisotropically; hydrogen atoms were refined as rigid groups. R values [$I > 2\sigma(I)$]: R_1 = 0.0235, wR_2 = 0.0557. R values [all data]: R_1 = 0.0290, wR_2 = 0.0574, min/max difference electron difference –2.141/1.484.

Complex 3b ($C_{21}H_{39}NO_6PSi_2W$): M = 672.53 monoclinic, $P2_1/c$ a = 14.7971(4) Å, b = 15.3781(4) Å, c = 12.4122(3) Å, V = 2811.70(13) Å^3, Z = 4; $d_{calc.}$ = 1.589 Mg/m^3, μ = 4.284 mm^{-1}, T = 123(2) K. A total 23804 reflections were measured on a Nonius KappaCCD diffractometer using monochromated Mo Kα radiation (λ = 0.71073 Å), 6783 reflections were unique (R_{int} = 0.0520). The structure was solved with Patterson methods and refined with full-matrix least-squares against F^2 of all reflections. Non-hydrogen atoms were refined anisotropically; hydrogen atoms were refined as rigid groups. R values [$I > 2\sigma(I)$]: R_1 = 0.0308, wR_2 = 0.0554. R values [all data]: R_1 = 0.0452, wR_2 = 0.0577, min/max difference electron difference –1.49/1.30.

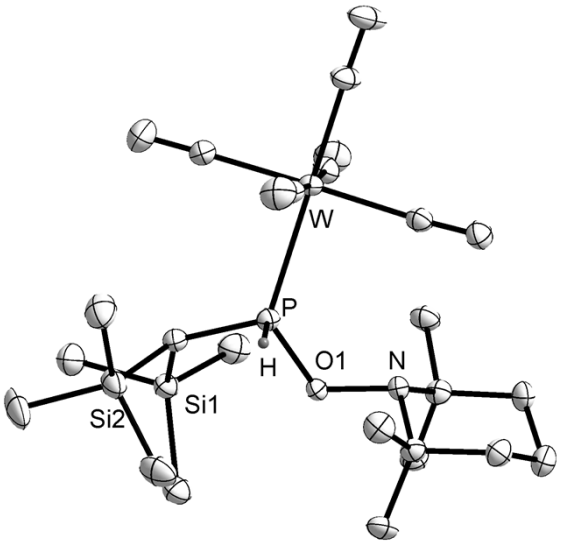

Fig. S1 Molecular structure of complex **3b** (50% probability level; hydrogen atoms are omitted for clarity). Selected bond lengths [Å] and angles [°]: W–P 2.5117(8), P–O(1) 1.656(2), P–C 1.827(4), O–P–W 125.37(9), C(1)–P–W 119.30(11).

Complex 5 ($C_{21}H_{39}FNO_6PSi_2W$): M = 691.52, triclinic, P-1, a = 9.1438(7), b = 12.12.6924(10) Å, c = 13.4939(11) Å, V = 1469.0(2) Å^3, Z = 2; $d_{calc.}$ = 1.559 Mg/m^3, μ = 4.106 mm^{-1}, T = 123(2) K. A total 48243 reflections were measured on a Nonius KappaCCD diffractometer using monochromated Mo Kα radiation (λ = 0.71073 Å), 6310 reflections were unique (R_{int} = 0.0701). A semiempirical absorption correction from equivalents was applied (min/max transmission 0.4653/0.7347). The structure was solved with Patterson methods and refined with full-matrix least-squares against F^2 of all reflections. Non-hydrogen atoms were refined anisotropically; hydrogen atoms were refined as rigid groups. R values [$I > 2\sigma(I)$]: R_1 = 0.0547, wR_2 = 0.1141. R values [all data]: R_1 = 0.0841, wR_2 = 0.1344, min/max difference electron difference –2.036/3.440.

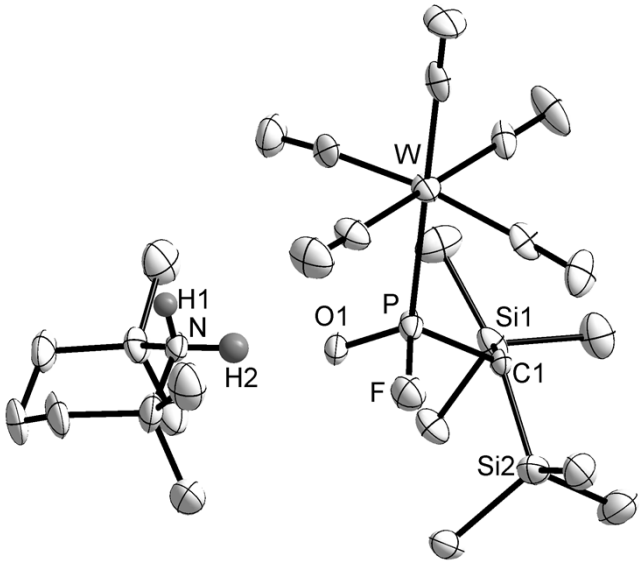

Fig. S2 Molecular structure of complex **5** (50% probability level; hydrogen atoms are omitted for clarity). Selected bond lengths [Å] and angles [°]: W–P 2.519(2), P–O(1) 1.489(6), P–F 1.658(6), P–C(1) 1.828(7), H2–O1 1.6865(1), O–P–W 122.8(3), F–P–W 104.3(2), C(1)–P–W 116.1(3).

C. Computational Details

The quantum chemical DFT calculations have been performed with the TURBOMOLE suite of programs.[1, 2] The structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO level of theory, which combines the accurate TPSS meta-GGA density functional[3] with the BJ-damped DFT-D3 dispersion correction[4, 5] and the def2-TZVP basis set,[6-8] using the Conductor-like Screening Model (COSMO) continuum solvation model [9] for THF solvent (dielectric constant $\varepsilon = 7.58$, refractive constant $n = 1.407$, $R_{solv} = 3.18$ Å). The density-fitting RI-J approach[10, 11] is used to accelerate the geometry optimization and numerical harmonic frequency calculations in solution. The 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 corrections according to the ideal gas–rigid rotor–harmonic oscillator model.[12]

To get better solvation free energies in both THF and toluene solvents, gas-phase single-point calculations are done at TPSS-D3 level of theory using larger def2-QZVP basis set[13], and the COSMO-RS solvation model in the COSMOtherm program package[14] is applied to the above TPSS-D3 optimized structures, and. The final Gibbs free energies (ΔG) are determined from gas-phase TPSS-D3/def2-QZVP energies plus thermal (298.15 K, 1 atm) and COSMO-RS solvation corrections. In our discussion, the final Gibbs free energies (in kcal mol^{-1}) will be used unless specified otherwise.

References

[1] R. Ahlrichs, M. Bär, M. Häser, H. Horn, C. Kölmel, *Chem. Phys. Lett.* **1989**, *162*, 165.
[2] R. Ahlrichs, M. K. Armbruster, R. A. Bachorz, M. Bär, H.-P. Baron, R. Bauernschmitt, F. A. Bischoff, S. Böcker, N. Crawford, P. Deglmann, F. D. Sala, M. Diedenhofen, M. Ehrig, K. Eichkorn, S. Elliott, F. Furche, A. Glöß, F. Haase, M. Häser, C. Hättig, A. Hellweg, S. Höfener, H. Horn, C. Huber, U. Huniar, M. Kattannek, W. Klopper, A. Köhn, C. Kölmel, M. Kollwitz, K. May, P. Nava, C. Ochsenfeld, H. Öhm, M. Pabst, H. Patzelt, D. Rappoport, O. Rubner, A. Schäfer, U. Schneider, M. Sierka, D. P. Tew, O. Treutler, B. Unterreiner, M. von Arnim, F. Weigend, P. Weis, H. Weiss, N. Winter in TURBOMOLE v6.4, TURBOMOLE GmbH, **2012**.
[3] J. M. Tao, J. P. Perdew, V. N. Staroverov, G. E. Scuseria *Phys. Rev. Lett.* **2003**, *91*, 146401.
[4] S. Grimme, S. Ehrlich, H. Krieg, D. 132 *J. Chem. Phys.* **2010**, *132*, 154104.
[5] S. Grimme, L. Goerigk, *J. Comput. Chem.* **2011**, *32*, 1456.
[6] A. Schaefer, C. Huber, R. Ahlrichs, *J. Chem. Phys.* **1994**, *100*, 5829.
[7] F. Weigend, M. Häser, H. Patzelt, R. Ahlrichs, *Chem. Phys. Lett.* **1998**, *143*, 294.
[8] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.
[9] A. Klamt; G. Schüürmann, *J. Chem. Soc. Perkin Trans.* 1993, *2*, 799.
[10] K. Eichkorn, F. Weigend, O. Treutler, R. Ahlrichs, *Theor. Chem. Acc.* **1997**, *97*, 119.
[11] P. Deglmann, K. May, F. Furche, R. Ahlrichs, *Chem. Phys. Lett.* **2004**, *384*, 103.
[12] S. Grimme, *Chem. Eur. J.* **2012**, ***18***, 9955
[13] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297.
[14] F. Eckert, A. Klamt, COSMOtherm, Version C2.1, Release 01.11; COSMOlogic GmbH & Co. KG, Leverkusen, Germany, 2010.

Table S1. The TPSS-D3/def2-TZVP + COSMO computed zero-point energies, enthalpy corrections, Gibs free energy corrections (ZPE, Hc and Gc, respectively, in kcal/mol), the COSMO-RS solvation enthalpies and free energies (Hcs and Gcs, respectively, in kcal/mol) in THF solvent, and the TPSS-D3/def2-QZVP single-point energies (Ee, in hartrees) for some crucial structures. For each structure, the number of atoms, the structure name and the total energy (in hartrees) are given followed by the Cartesian coordinates of each atom (in angstroms). Some structures derived from named neutral species such as the cation, anion, H-added, H-abstracted, and silyl-abstracted are named simply by adding the corresponding +, **–**, **H**, **mH** and **mS** suffixes to the neutral name.

NAME	ZPE	Hc	Gc	Hcs	Gcs	Ee
1a	330.44	360.96	284.77	-38.25	-24.59	-2556.576343
2a	176.26	197.41	139.22	-15.29	-5.39	-1933.202585
2a-	175.42	196.66	138.26	-50.02	-38.87	-1933.299973
2aH	182.69	203.91	145.47	-15.97	-5.94	-1933.841892
3a	340.25	369.34	296.74	-21.24	-10.34	-2417.332654
3a-	338.71	367.88	295.14	-57.84	-45.45	-2417.356142
3amS	268.80	293.33	229.21	-20.19	-9.74	-2007.864946
3amS-	268.15	292.56	228.82	-52.27	-40.72	-2007.967254
4	333.37	364.39	287.23	-36.55	-23.20	-2631.940354
5	355.21	384.93	310.85	-26.78	-14.79	-2418.631401
6	249.33	275.96	207.48	-17.58	-6.88	-2418.015379
7	179.14	200.80	141.76	-15.95	-5.92	-2008.509128
7-	178.40	200.14	140.80	-50.37	-39.38	-2008.645567
7H	186.02	207.95	148.38	-27.54	-10.33	-2009.152724
7H-TEMPH2+	291.37	316.70	250.29	-25.67	-14.40	-2009.812807
CPh_3	172.01	181.83	147.71	-20.45	-10.59	-733.526090
CPh_3+	173.28	183.09	148.99	-54.84	-42.50	-733.312098
H	0.00	1.48	-6.69	-1.07	5.38	-0.500161
$PhCH_2$	71.31	75.42	53.55	-9.27	-1.92	-271.095262
$PhCH_3$	79.41	83.73	60.95	-9.08	-1.84	-271.745709
TEMP	158.36	166.00	136.60	-11.52	-3.82	-408.781888
TEMP-	155.63	163.01	134.12	-58.12	-48.90	-408.804730
TEMPH	166.18	174.03	144.19	-11.93	-3.92	-409.438043
$TEMPH_2$+	176.23	183.94	154.44	-71.11	-51.42	-409.832862
TEMPO	161.86	169.99	139.57	-12.57	-4.77	-484.046161
TEMPO-	159.58	167.78	137.27	-60.33	-51.13	-484.053155
TEMPO+	162.84	170.88	140.67	-55.73	-44.27	-483.800897
TEMPOH	168.74	177.01	146.48	-17.46	-6.06	-484.657942
THF	72.21	75.88	54.79	-7.25	-0.66	-232.603972
THFmH	63.79	67.40	46.57	-7.40	-0.75	-231.948301

Table S2. The TPSS-D3/def2-TZVP + COSMO(THF) optimized geometries for some crucial structures. For each structure, the number of atoms, the structure name and the total energy (in hartrees) are given followed by the Cartesian coordinates of each atom (in angstroms). Some structures derived from named neutral species such as the cation, anion, H-added, H-abstracted, and silyl-abstracted are named simply by adding the corresponding **+**, **–**, **H**, **mH** and **mS** suffixes to the neutral name.

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70
1a Energy = -2556.472162664
P    -0.0244626    1.0131212   -0.4216000
F    -0.5445287    1.9149732    0.8938731
C     2.7729609    3.5885529   -3.0772626
W     1.5902340    2.4886487   -1.8801162
C     0.0709796    2.9968888   -3.1635640
C     3.2993332    2.1678010   -0.7896497
C     1.9095035    0.7364851   -2.8884427
C     1.1675268    4.0271172   -0.5845399
O    -0.7276397    3.3150706   -3.9438720
O     2.0934568   -0.2840532   -3.4139649
O     4.3358768    2.0999190   -0.2666577
O     0.9508220    4.8531314    0.1986449
O     3.4425053    4.2382115   -3.7801073
C    -1.6422457    0.8649275   -1.3531652
Si   -2.2152101   -0.9435679   -1.3482592
Si   -2.9653475    2.1720402   -0.9453010
C    -3.7894510   -1.1982256   -2.3642651
C    -0.8717934   -1.9865757   -2.1649456
C    -2.5607407   -1.5807179    0.3893972
C    -4.1221299    2.3139153   -2.4336179
C    -3.9674259    1.6878445    0.5776594
C    -2.2930200    3.9079193   -0.6559798
Li    1.1126849   -0.8146727    0.9620690
H    -1.4026510    1.0805087   -2.4046695
H    -3.9897072   -2.2738575   -2.4568776
H    -4.6653408   -0.7389747   -1.8924292
H    -3.6958483   -0.7885537   -3.3767262
H    -1.1679108   -3.0432329   -2.1955114
H    -0.7057154   -1.6563932   -3.1979010
H     0.0850125   -1.9202987   -1.6372290
H    -2.7169390   -2.6671793    0.3603079
H    -1.7354700   -1.3845735    1.0790894
H    -3.4666635   -1.1274417    0.8045197
H    -4.8612464    3.1043892   -2.2486933
H    -3.5593280    2.5909308   -3.3333354
H    -4.6658938    1.3895809   -2.6476986
H    -4.6409261    2.5085255    0.8555417
H    -4.5834336    0.7988771    0.4018451
H    -3.3094695    1.4848565    1.4297049
H    -3.1456687    4.5946414   -0.5662533
H    -1.7021948    3.9704122    0.2601755
H    -1.6729498    4.2598854   -1.4857066
O     1.5614259   -2.7624258    0.2254382
O     1.6828148    0.1834099    2.7609581
O     0.1292489   -2.0008941    2.3953555
O     3.1318699   -0.6044544    0.6154958
C     1.5043436   -0.6897537    3.8888015
C     2.9813586   -2.9929605    0.3080014
C     0.6404875   -3.3456094    2.3892134
C     0.7615629   -3.7335679    0.9275116
C     0.1566485   -1.3510311    3.6819214
C     3.0278089    0.6708479    2.5952873
C     3.6322200   -1.7071270   -0.1625500
C     3.8583296   -0.3416464    1.8285966
H     1.5171968   -0.1111035    4.8216768
H     2.3092606   -1.4363073    3.9285958
H     1.6145650   -3.3852705    2.8950114
H     3.2624539   -3.8369065   -0.3345343
H     3.2694974   -3.2257506    1.3417378
H     1.1872583   -4.7374766    0.8210564
H    -0.6311834   -0.5943787    3.6441818
H    -0.2193151   -3.7057776    0.4479466
H     3.9888702   -1.2689752    2.4028786
H    -0.0536367   -4.0150955    2.9132811
H    -0.0650895   -2.0655759    4.4820213
H     3.3460065   -1.4940340   -1.1951758
H     3.4830031    0.8957248    3.5665052
H     2.9323018    1.5935087    2.0199948
H     4.7238579   -1.7676537   -0.0957973
H     4.8472897    0.0694276    1.5921033

42
2aH Energy = -1933.757640064
W     0.1134720    3.3669745   -0.1852174
Si   -0.1741685   -1.7290760   -1.5040364
Si   -0.0419685   -0.9685629    1.6603987
P     0.9220872    1.0232024   -0.4428463
O     2.6721972    4.3096664   -1.8951190
O     1.8235547    3.7903581    2.5066719
O    -1.5456724    2.8984278   -2.9010509
O    -2.4304895    2.3296816    1.4787504
O    -0.9402525    6.3779579   -0.0129738
F     1.5114967    0.8139435   -1.9451879
C     1.5590933   -2.3908808   -1.8021018
C     1.2310801   -2.3454516    1.7881075
C     0.5191154    0.4129689    2.8133812
C    -0.8864597   -0.9927238   -3.0816322
C     1.7543102    3.9725745   -1.2813634
C    -0.2007988   -0.3538628   -0.1585341
C    -1.3072480   -3.1328389   -0.9659735
C     1.2048298    3.6321767    1.5443021
C    -1.7443664   -1.5338679    2.2156091
C    -0.9496250    3.0709297   -1.9265359
C    -1.5117982    2.7116094    0.8883629
C    -0.5587771    5.2859946   -0.0709985
H     1.3405247   -2.6308114    2.8417793
H     0.9485759   -3.2420682    1.2278314
H     1.9914853   -2.8414136   -0.9034126
H     2.2142513   -2.0164297    1.4321238
H     1.5143214   -3.1692733   -2.5742318
H     2.2380030   -1.6084390   -2.1547270
H     1.5082908    0.8100588    2.5609640
H    -0.9802794   -1.7701029   -3.8500224
H    -0.2561771   -0.1932551   -3.4825911
H     0.5896001   -0.0012594    3.8275780
H    -1.3626061   -3.8675656   -1.7794822
H    -0.9508547   -3.6559307   -0.0728942
H    -1.7069571   -1.8354980    3.2695635
H    -0.1865826    1.2479887    2.8487768
H    -1.8865181   -0.5796038   -2.9027007
H    -2.1169089   -2.3825153    1.6348673
H    -1.2116410    0.0742674   -0.2331392
H    -2.3252306   -2.7767177   -0.7716900
H    -2.4696356   -0.7163373    2.1281886
H     2.0887270    0.6057048    0.2312060

41
2a- Energy = -1933.257421243
W     0.1872920    3.3904295   -0.1441306
Si   -0.1452591   -1.6341313   -1.4756898
```

Si	-0.0066837	-0.9104125	1.6326199
P	1.2177192	0.9692437	-0.3591637
O	2.7895962	4.2425819	-1.8301358
O	1.8319045	3.8588700	2.5771762
O	-1.3332797	2.6001693	-2.8619531
O	-2.3134667	2.1836642	1.4637046
O	-1.0037532	6.3364228	-0.1228770
F	1.4721969	0.8814904	-2.0332032
C	1.5800726	-2.3141788	-1.8162115
C	1.2684433	-2.2958251	1.7704681
C	0.5519385	0.4319655	2.8394303
C	-0.8826568	-0.9551497	-3.0729633
C	1.8439235	3.9500016	-1.2223376
C	-0.1560553	-0.2741632	-0.1521512
C	-1.2575245	-3.0808155	-0.9672715
C	1.2301010	3.6907303	1.5963444
C	-1.6921246	-1.5184386	2.2288789
C	-0.7850825	2.9018206	-1.8848477
C	-1.4032797	2.6385456	0.8994384
C	-0.5546692	5.2544140	-0.1168495
H	1.3894693	-2.5798881	2.8236670
H	0.9863808	-3.1945668	1.2120121
H	2.0230408	-2.7754096	-0.9276494
H	2.2428068	-1.9565534	1.3999867
H	1.5245790	-3.0812019	-2.5998184
H	2.2515733	-1.5213398	-2.1595521
H	1.5004820	0.8849015	2.5310038
H	-0.9417778	-1.7448867	-3.8333735
H	-0.2812469	-0.1317381	-3.4677087
H	0.7032278	-0.0226706	3.8278548
H	-1.3033322	-3.8054757	-1.7912366
H	-0.8938686	-3.6103300	-0.0801264
H	-1.6341727	-1.8203472	3.2826355
H	-0.1853026	1.2325933	2.9484653
H	-1.8982724	-0.5769860	-2.9029242
H	-2.0580456	-2.3735421	1.6519647
H	-1.1486690	0.1907234	-0.2515022
H	-2.2815321	-2.7453591	-0.7638830
H	-2.4346925	-0.7151581	2.1519092

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2a Energy = -1933.117713405

W	0.1669731	3.4019115	-0.2142369
Si	-0.1666955	-1.6808870	-1.4943615
Si	0.0686624	-1.0026395	1.7069338
P	0.9414501	1.0560189	-0.3635549
O	2.8207080	4.3623261	-1.7678652
O	1.6202877	4.0075468	2.5991041
O	-1.2592780	2.8456530	-3.0445466
O	-2.4052083	2.2740059	1.3401249
O	-1.0933481	6.3356451	-0.2615004
F	1.7130918	0.7371842	-1.7651116
C	1.5256969	-2.4298517	-1.8177659
C	1.3587349	-2.3655486	1.7850530
C	0.6209262	0.3954985	2.8424016
C	-0.8279336	-0.8564463	-3.0501615
C	1.8687552	4.0220939	-1.2126130
C	-0.1440142	-0.3603269	-0.1007419
C	-1.3626630	-3.0436924	-0.9886453
C	1.1026730	3.7776466	1.5943270
C	-1.6117996	-1.6028954	2.2960621
C	-0.7490978	3.0454847	-2.0294862
C	-1.4838906	2.6988193	0.7852916
C	-0.6207335	5.2794059	-0.2296368
H	1.5181273	-2.6518473	2.8320125
H	1.0542426	-3.2632943	1.2372153
H	1.9266450	-2.9421023	-0.9379139
H	2.3205687	-2.0282276	1.3820287
H	1.4334990	-3.1727427	-2.6203305
H	2.2520139	-1.6772481	-2.1376824
H	1.6007699	0.7984830	2.5626376
H	-0.9601793	-1.6022395	-3.8437510
H	-0.1466438	-0.0850278	-3.4229051
H	0.7019801	0.0083355	3.8661777
H	-1.4742023	-3.7443674	-1.8259563
H	-1.0073553	-3.6158836	-0.1250792
H	-1.5453143	-1.9080846	3.3476921
H	-0.0954875	1.2234736	2.8602663
H	-1.8025970	-0.3890523	-2.8662626
H	-1.9823361	-2.4559958	1.7204780
H	-1.1662847	0.0546716	-0.1150923
H	-2.3563295	-2.6470383	-0.7519656
H	-2.3544136	-0.7987648	2.2293604

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3amS Energy = -2007.909292004

P	1.3060977	0.7686921	0.6227878
O	-0.3083803	0.3474866	0.4402874
N	-0.8795219	0.3286159	-0.9035009
C	4.0098214	2.2664999	-2.7352475
W	2.7268443	1.6122926	-1.3313796
C	4.1441088	1.9125630	0.1235376
C	1.3325255	1.3280565	-2.8254705
C	2.0300299	3.5181562	-1.0088961
C	3.3664599	-0.3310583	-1.5442583
O	4.9629724	2.0931217	0.9248637
O	1.6561051	4.5989760	-0.8205063
O	0.6412296	1.2101352	-3.7489814
O	3.7410337	-1.4212088	-1.6598457
O	4.7671262	2.6511837	-3.5386733
F	0.8966631	2.1048572	1.5471749
C	1.9925040	-0.3966030	1.6140608
Si	1.2570528	-1.3281211	2.9963485
H	3.0501831	-0.5363052	1.3908911
C	0.8093246	-3.1185335	2.5381053
C	2.4960326	-1.4643207	4.4287739
C	-0.3152243	-0.5042489	3.6535723
H	2.0980879	-2.0688034	5.2551316
H	3.4298340	-1.9337027	4.0920785
H	2.7482618	-0.4718727	4.8215870
H	0.4076252	-3.6717741	3.3984595
H	0.0619047	-3.1451803	1.7370405
H	1.6966246	-3.6544594	2.1765697
H	-0.7518189	-1.0847633	4.4769122
H	-0.0983294	0.5056206	4.0214675
H	-1.0662477	-0.4098938	2.8614856
C	-2.0086568	1.3130802	-0.8978273
C	-2.7094312	1.2008042	-2.2662575
C	-3.0141217	1.1465796	0.2601758
C	-1.3814910	2.7089967	-0.7930982
C	-3.1376351	-0.2251445	-2.6039977
H	-3.5675864	1.8839532	-2.2582593
H	-2.0145220	1.5554372	-3.0372738
C	-1.9085088	-1.1305445	-2.5707455
H	-3.8960700	-0.5779131	-1.8940625
H	-3.6004442	-0.2539717	-3.5978209
C	-1.1823423	-1.1068613	-1.2115933
H	-2.1740228	-2.1720894	-2.7890911
H	-1.2029713	-0.8020063	-3.3434843
C	-2.0028373	-1.8453388	-0.1339298
C	0.1676273	-1.8182498	-1.3672214
H	-3.6287060	2.0512078	0.3291074
H	-3.6849953	0.2966512	0.1205671
H	-2.4767870	1.0206381	1.2032703
H	-1.6062303	-1.6187506	0.8577391
H	-3.0629651	-1.5850128	-0.1575371
H	-1.9195432	-2.9249950	-0.3007184
H	-2.1633966	3.4693420	-0.9013451

H	-0.8872445	2.8470310	0.1705183
H	-0.6430236	2.8486467	-1.5864503
H	-0.0005049	-2.8584950	-1.6690705
H	0.7652501	-1.3215157	-2.1360790
H	0.7322300	-1.8068877	-0.4298906

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3amS Energy = -2007.909292004

P	1.3060977	0.7686921	0.6227878
O	-0.3083803	0.3474866	0.4402874
N	-0.8795219	0.3286159	-0.9035009
C	4.0098214	2.2664999	-2.7352475
W	2.7268443	1.6122926	-1.3313796
C	4.1441088	1.9125630	0.1235376
C	1.3325255	1.3280565	-2.8254705
C	2.0300299	3.5181562	-1.0088961
C	3.3664599	-0.3310583	-1.5442583
O	4.9629724	2.0931217	0.9248637
O	1.6561051	4.5989760	-0.8205063
O	0.6412296	1.2101352	-3.7489814
O	3.7410337	-1.4212088	-1.6598457
O	4.7671262	2.6511837	-3.5386733
F	0.8966631	2.1048572	1.5471749
C	1.9925040	-0.3966030	1.6140608
Si	1.2570528	-1.3281211	2.9963485
H	3.0501831	-0.5363052	1.3908911
C	0.8093246	-3.1185335	2.5381053
C	2.4960326	-1.4643207	4.4287739
C	-0.3152243	-0.5042489	3.6535723
H	2.0980879	-2.0688034	5.2551316
H	3.4298340	-1.9337027	4.0920785
H	2.7482618	-0.4718727	4.8215870
H	0.4076252	-3.6717741	3.3984595
H	0.0619047	-3.1451803	1.7370405
H	1.6966246	-3.6544594	2.1765697
H	-0.7518189	-1.0847633	4.4769122
H	-0.0983294	0.5056206	4.0214675
H	-1.0662477	-0.4098938	2.8614856
C	-2.0086568	1.3130802	-0.8978273
C	-2.7094312	1.2008042	-2.2662575
C	-3.0141217	1.1465796	0.2601758
C	-1.3814910	2.7089967	-0.7930982
C	-3.1376351	-0.2251445	-2.6039977
H	-3.5675864	1.8839532	-2.2582593
H	-2.0145220	1.5554372	-3.0372738
C	-1.9085088	-1.1305445	-2.5707455
H	-3.8960700	-0.5779131	-1.8940625
H	-3.6004442	-0.2539717	-3.5978209
C	-1.1823423	-1.1068613	-1.2115933
H	-2.1740228	-2.1720894	-2.7890911
H	-1.2029713	-0.8020063	-3.3434843
C	-2.0028373	-1.8453388	-0.1339298
C	0.1676273	-1.8182498	-1.3672214
H	-3.6287060	2.0512078	0.3291074
H	-3.6849953	0.2966512	0.1205671
H	-2.4767870	1.0206381	1.2032703
H	-1.6062303	-1.6187506	0.8577391
H	-3.0629651	-1.5850128	-0.1575371
H	-1.9195432	-2.9249950	-0.3007184
H	-2.1633966	3.4693420	-0.9013451
H	-0.8872445	2.8470310	0.1705183
H	-0.6430236	2.8486467	-1.5864503
H	-0.0005049	-2.8584950	-1.6690705
H	0.7652501	-1.3215157	-2.1360790
H	0.7322300	-1.8068877	-0.4298906

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3a- Energy = -2417.285112265

P	0.8551753	0.6366677	-0.0193257
O	-0.7426310	0.1782299	0.1272817
N	-1.4974225	0.5182405	-1.1228871
C	3.6691607	2.2535603	-3.4629466
W	2.4257945	1.4797477	-2.1494666
C	3.9159808	0.9188847	-0.8560375
C	0.7761419	1.9476093	-3.2787011
C	2.2817164	3.3133002	-1.2379795
C	2.5298450	-0.2901480	-3.1818713
O	4.7723166	0.5951078	-0.1114033
O	2.2099715	4.3817134	-0.7638366
O	-0.1373714	2.2273257	-3.9608544
O	2.6240005	-1.2433158	-3.8614691
O	4.4181793	2.7224878	-4.2375567
F	0.7518154	2.0672889	0.7765939
C	1.6092185	-0.2950500	1.3727205
Si	1.0283091	0.2679545	3.1101060
Si	1.8605954	-2.1622590	1.1061240
H	2.6457914	0.0838683	1.3122686
C	1.4310760	-0.9944750	4.4597778
C	1.9666106	1.8320151	3.5899252
C	-0.8291645	0.5517113	3.1988362
C	3.2251896	-2.7852448	2.2551812
C	0.2668635	-3.1085739	1.4422851
C	2.5068354	-2.5296297	-0.6210072
H	0.4166489	-4.1830298	1.2795088
H	-0.0702271	-2.9692124	2.4758298
H	-0.5415664	-2.7756777	0.7845701
H	3.5662404	-3.7632545	1.8912801
H	4.0883650	-2.1085303	2.2363380
H	2.9096572	-2.9066318	3.2939613
H	2.6004843	-3.6160812	-0.7501986
H	1.8794132	-2.1440720	-1.4249208
H	3.5023936	-2.0888943	-0.7462089
H	1.7022280	2.1361483	4.6109659
H	3.0489120	1.6513684	3.5674929
H	1.7494873	2.6614449	2.9116525
H	1.0362945	-0.6012882	5.4064629
H	0.9719785	-1.9746796	4.2939972
H	2.5092583	-1.1375130	4.5853841
H	-1.1131633	0.7795082	4.2343679
H	-1.1431333	1.3822079	2.5617012
H	-1.3815584	-0.3395680	2.8812123
C	-2.5431073	1.5282226	-0.7723492
C	-3.3123467	1.8050722	-2.0838580
C	-3.5031465	1.1316224	0.3671414
C	-1.8371637	2.8323235	-0.3783160
C	-3.8695763	0.5451579	-2.7386196
H	-4.1113650	2.5181981	-1.8478944
H	-2.6226565	2.2955744	-2.7808196
C	-2.7209145	-0.4250952	-2.9954586
H	-4.6309858	0.0811781	-2.0991320
H	-4.3661345	0.8004858	-3.6822746
C	-1.9427308	-0.7806194	-1.7124331
H	-3.0793289	-1.3633358	-3.4358081
H	-2.0175250	0.0287199	-3.7040082
C	-2.7790600	-1.6842919	-0.7819211
C	-0.6787982	-1.5404811	-2.1224228
H	-4.0213638	2.0302722	0.7202090
H	-4.2607155	0.4112298	0.0536590
H	-2.9413786	0.7105975	1.2040462
H	-2.3639818	-1.6736387	0.2289638
H	-3.8279297	-1.3862440	-0.7302688
H	-2.7416565	-2.7127561	-1.1576935
H	-2.5657739	3.6501194	-0.4107894
H	-1.4265092	2.7778139	0.6303931
H	-1.0226933	3.0501953	-1.0746177
H	-0.9450436	-2.3627472	-2.7954524
H	0.0187798	-0.8681670	-2.6290462
H	-0.1826053	-1.9686684	-1.2503831

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3a Energy = -2417.217145369

P	0.9167035	0.7268335	0.0402320
O	-0.6256118	0.1982459	0.0150634
N	-1.4321695	0.5475704	-1.2150380
C	3.4674818	2.2108272	-3.4339727
W	2.2722245	1.4306133	-2.0066002
C	3.9229508	0.9582237	-0.8831250
C	0.6219200	1.8556312	-3.1802499
C	2.2027510	3.3340207	-1.2134964
C	2.4425671	-0.3432261	-3.0363093
O	4.8570223	0.6822332	-0.2564724
O	2.1964934	4.4230950	-0.8310829
O	-0.2262228	2.1188178	-3.9179429
O	2.5910042	-1.2641415	-3.7203287
O	4.1647713	2.6751312	-4.2373715
F	0.7584197	2.1163355	0.8760134
C	1.6267456	-0.2728072	1.3754630
Si	0.9923943	0.2317880	3.1370223
Si	1.8898280	-2.1533400	1.1076948
H	2.6658488	0.1034156	1.3723832
C	1.3701063	-1.0712265	4.4463990
C	1.9240381	1.7756773	3.6794779
C	-0.8646237	0.5039212	3.1574858
C	3.2640845	-2.7203730	2.2675676
C	0.2974377	-3.0998529	1.4203868
C	2.5477097	-2.5572584	-0.6059204
H	0.4809814	-4.1776389	1.3336668
H	-0.1084609	-2.9082997	2.4192026
H	-0.4734914	-2.8320357	0.6918359
H	3.6333601	-3.6895001	1.9091683
H	4.1093923	-2.0214471	2.2485241
H	2.9505968	-2.8467551	3.3053026
H	2.7775776	-3.6304016	-0.6339577
H	1.8508119	-2.3505886	-1.4181771
H	3.4790520	-2.0176896	-0.8102273
H	1.6609903	2.0205806	4.7162376
H	3.0072678	1.6029255	3.6478332
H	1.6999835	2.6431536	3.0536061
H	0.9256083	-0.7085538	5.3829943
H	0.9405471	-2.0559311	4.2397614
H	2.4443760	-1.1894824	4.6176533
H	-1.1917430	0.6663510	4.1919553
H	-1.1577024	1.3750194	2.5663682
H	-1.4000307	-0.3684054	2.7670073
C	-2.4647471	1.5674205	-0.8234086
C	-3.2947378	1.8199277	-2.1045252
C	-3.3791732	1.1885998	0.3569681
C	-1.7507359	2.8804820	-0.4784350
C	-3.8965817	0.5514328	-2.6982554
H	-4.0737509	2.5437682	-1.8392433
H	-2.6446995	2.2954480	-2.8478679
C	-2.7736820	-0.4372055	-2.9892182
H	-4.6299147	0.1126018	-2.0111606
H	-4.4363196	0.7895195	-3.6216439
C	-1.9251383	-0.7681561	-1.7432104
H	-3.1633768	-1.3852454	-3.3773154
H	-2.1106638	-0.0165413	-3.7547386
C	-2.7168976	-1.6346180	-0.7424247
C	-0.7005303	-1.5543761	-2.2116206
H	-3.8612625	2.0995462	0.7273182
H	-4.1658890	0.4869378	0.0775129
H	-2.7971683	0.7576881	1.1730660
H	-2.2553105	-1.6024614	0.2468456
H	-3.7590424	-1.3266435	-0.6490067
H	-2.7066055	-2.6724031	-1.0912641
H	-2.4798766	3.6958399	-0.5230838
H	-1.3290111	2.8602730	0.5262426
H	-0.9508240	3.0893401	-1.1943146
H	-1.0244749	-2.4435691	-2.7610296
H	-0.0849157	-0.9368836	-2.8681473
H	-0.0976615	-1.8821776	-1.3640727

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4 Energy = -2631.828444774

P	-0.2844543	1.4597755	-0.4895756
F	-0.9916336	2.2553326	0.7614974
C	2.8510879	3.9285020	-2.7361834
W	1.4244368	2.9152172	-1.7251352
C	0.1508309	3.1425474	-3.3193659
C	2.6964263	2.7360492	-0.1220279
C	2.0675878	1.1119984	-2.4710864
C	0.7202237	4.6371211	-0.8473764
O	-0.5548709	3.2747574	-4.2303099
O	2.4261043	0.0866873	-2.8749796
O	3.4358647	2.6910594	0.7687595
O	0.3515692	5.6036151	-0.3268816
O	3.6793956	4.5044707	-3.3192210
O	0.2887387	0.2035036	0.1496328
C	-1.7812334	1.0249866	-1.4603603
Si	-2.2380784	-0.8190093	-1.2705971
Si	-3.2256795	2.2649815	-1.3679905
C	-3.8150324	-1.2062182	-2.2434506
C	-0.8826132	-1.8600686	-2.0651789
C	-2.5520187	-1.3207197	0.5145918
C	-4.1798689	2.1930090	-2.9953106
C	-4.3659257	1.8626895	0.0774811
C	-2.6764310	4.0576183	-1.1789827
Li	1.3703680	-0.8429670	1.1609777
H	-1.4363002	1.0950551	-2.5050357
H	-4.0022493	-2.2871091	-2.1879403
H	-4.7001526	-0.6984678	-1.8453028
H	-3.7190589	-0.9413413	-3.3027593
H	-1.1533358	-2.9240281	-2.0489030
H	-0.7554477	-1.5702230	-3.1163677
H	0.0768144	-1.7341032	-1.5581939
H	-2.8727811	-2.3703380	0.5520892
H	-1.6529308	-1.2106915	1.1243911
H	-3.3490306	-0.7153167	0.9600909
H	-4.9686006	2.9563142	-2.9926765
H	-3.5124903	2.4104239	-3.8384779
H	-4.6508328	1.2235472	-3.1790378
H	-5.1568701	2.6197266	0.1508432
H	-4.8491503	0.8854772	-0.0294172
H	-3.8072552	1.8648165	1.0202194
H	-3.5683629	4.6972275	-1.2185858
H	-2.1694135	4.2402742	-0.2286532
H	-2.0099782	4.3734602	-1.9877097
O	1.6843154	-2.7477763	0.2259246
O	2.0758955	-0.1945319	3.1200122
O	0.2751060	-2.1503944	2.4769444
O	3.4785792	-0.7870413	0.8478299
C	1.7739217	-1.1855579	4.1178507
C	3.0753724	-3.1068735	0.2541241
C	0.7000215	-3.5119007	2.3039194
C	0.8027260	-3.7261575	0.8055098
C	0.3646685	-1.6630658	3.8273082
C	3.4775453	0.1308678	3.0288932
C	3.8392211	-1.8365445	-0.0707489
C	4.1822358	-0.8402444	2.1009358
H	1.8345620	-0.7423035	5.1207084
H	2.4914044	-2.0153653	4.0603840
H	1.6686698	-3.6783029	2.7949602
H	3.2815460	-3.8833368	-0.4946406
H	3.3507731	-3.4966591	1.2435465
H	1.1434349	-4.7426219	0.5769976
H	-0.3352190	-0.8251226	3.8814850

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H    -0.1691130   -3.5579973    0.3363759
H     4.1620140   -1.8607590    2.5073456
H    -0.0360468   -4.1974241    2.7449604
H     0.0577233   -2.4358430    4.5419431
H     3.5514472   -1.4695840   -1.0582053
H     3.9416055    0.1232256    4.0220418
H     3.5193065    1.1406748    2.6191171
H     4.9208197   -2.0143907   -0.0504288
H     5.2300965   -0.5446130    1.9574062

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5  Energy = -2418.519221492
W     3.1226748    1.2422972   -1.4698775
P     1.3644752    0.5761503    0.2653224
O     0.0747213   -0.1331655   -0.1615651
H    -0.9870727    0.3624260   -1.1589750
N    -1.7890151    0.6297277   -1.8408269
H    -1.3975722    1.3368835   -2.4726730
F     0.8338086    2.0282341    0.8424820
O     0.5896535    2.6053213   -2.8863048
O     2.7049697   -1.3242888   -3.3543644
O     3.6758952    3.8198320    0.3764770
O     5.2301949    2.3538868   -3.5897498
O     5.3214930   -0.4258769    0.1783101
Si    1.2181835    0.5028591    3.3980081
Si    1.7943872   -2.1315160    1.6088060
C     0.0710834   -2.7240335    2.0810755
C    -0.6518625    0.6976996    3.3108751
C    -0.8637434   -0.7871982   -3.5824504
C     1.5354388    2.1469098   -2.3878433
C     1.6258400   -0.5950333    4.8794455
C     1.9413516   -0.2345132    1.7911109
C     2.0463898    2.1640360    3.7258053
C    -2.1041748   -0.5958600   -2.7046836
C     2.1482875   -2.7132034   -0.1482003
C    -2.2898052   -1.8327101   -1.8190518
C    -2.3024392    2.6722000   -0.6217370
C     2.8314346   -0.4095917   -2.6542436
C    -2.9007067    1.3275631   -1.0502252
C     3.1048181   -2.9334327    2.7037872
C    -3.2554830    0.5059777    0.1934785
C    -3.3424134   -0.2802855   -3.5534295
C     3.4679580    2.8946583   -0.2849632
C    -4.0980060    1.5349231   -1.9878816
C     4.4664864    1.9360064   -2.8183254
C    -4.5124714    0.2579758   -2.7247132
C     4.5476504    0.1884097   -0.4263330
H     0.0146829   -0.9919207   -2.9650863
H    -0.0129129   -3.8048002    1.9114091
H    -0.1701855   -2.5318543    3.1319566
H    -0.6699031    0.1001383   -4.1958527
H    -0.6750686   -2.2185131    1.4590008
H    -0.9412756    1.4232574    2.5458861
H    -1.0217928   -1.6355340   -4.2536303
H    -1.0309436    1.0487959    4.2790488
H     1.1570082   -1.5829373    4.8242755
H    -1.1459424   -0.2519488    3.0810829
H     1.2576261   -0.1036651    5.7897359
H     1.4154916   -2.3224800   -0.8589702
H    -1.4337666    2.5278200    0.0264933
H    -1.4760430   -1.9095034   -1.0929335
H     1.6967251    2.5819815    4.6784111
H     1.8366384    2.8877185    2.9333804
H    -1.9991299    3.2638820   -1.4930675
H     2.1027348   -3.8099372   -0.1747308
H    -2.2672672   -2.7162719   -2.4633255
H    -2.3486879    0.1839395    0.7116516
H     2.7065881   -0.7364527    4.9938421
H     2.9505766   -2.7436571    3.7696782
H     3.0205925   -0.0255108    1.8551659
H    -3.0582811    3.2406574   -0.0728955
H    -3.0682229    0.4642253   -4.3135612
H     3.0983180   -4.0201633    2.5506096
H     3.1349133    2.0445675    3.7966799
H     3.1471472   -2.4170973   -0.4855452
H    -3.2416746   -1.8331466   -1.2865852
H    -3.6264690   -1.1929592   -4.0878920
H    -3.8376044    2.3061789   -2.7259774
H    -3.8341250    1.1429117    0.8684431
H    -3.8622120   -0.3700967   -0.0393867
H     4.1038617   -2.5673834    2.4362614
H    -4.8591150   -0.5003579   -2.0132006
H    -4.9270547    1.9307237   -1.3917596
H    -5.3576568    0.4761246   -3.3851779

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6  Energy = -2417.906906436
P    -0.7812401   -0.1742970   -0.5566278
O    -0.5559944    1.0724838    0.4124519
C    -4.5826376   -2.6539723   -0.6523582
W    -2.8868143   -1.5373556   -0.5250944
C    -1.8206595   -3.2011855    0.0417426
C    -3.9210218    0.1424273   -1.1179103
C    -2.4506946   -1.9659605   -2.4930493
C    -3.3087777   -1.1407418    1.4531648
O    -1.2155357   -4.1387355    0.3471505
O    -2.2002335   -2.2142087   -3.5931253
O    -4.5053056    1.0796881   -1.4602452
O    -3.5683439   -0.9506337    2.5627604
O    -5.5492426   -3.2873083   -0.7383848
F    -0.7472535    0.5880535   -1.9915348
C     0.8041232   -1.0122850   -0.4772865
Si    2.1287717   -0.3468411   -1.7021697
Si    1.4073703   -1.2332009    1.3392428
H     0.5901134   -2.0357157   -0.8237134
C     3.7859194   -1.1811909   -1.3736943
C     1.6229432   -0.8330328   -3.4488275
C     2.3189926    1.5171580   -1.5478013
C     2.3444681   -2.8626672    1.4077842
C     2.4953992    0.2033720    1.8733000
C    -0.0123208   -1.3521699    2.5707826
H     2.7993715    0.0523692    2.9166537
H     3.4049429    0.3023458    1.2732675
H     1.9458291    1.1478364    1.8179668
H     2.6672519   -3.0585325    2.4378549
H     1.6978614   -3.6924465    1.0984696
H     3.2330662   -2.8694151    0.7702661
H     0.4177600   -1.5109800    3.5683089
H    -0.6129204   -0.4393786    2.6097925
H    -0.6792072   -2.1947962    2.3657188
H     2.4185707   -0.5636199   -4.1547260
H     1.4719968   -1.9173297   -3.5193419
H     0.7009205   -0.3406296   -3.7692587
H     4.5035831   -0.8242885   -2.1237793
H     4.2028285   -0.9608635   -0.3864566
H     3.7127351   -2.2695205   -1.4794702
H     3.1231300    1.8583471   -2.2114078
H     1.4011386    2.0387318   -1.8348905
H     2.5772842    1.8171740   -0.5274079
Si   -1.2121782    2.6037685    0.7538755
C    -2.7407553    2.3809791    1.8041995
H    -3.5440224    1.8721954    1.2622679
H    -2.5229800    1.8066096    2.7110596
H    -3.1195322    3.3636090    2.1121118
C     0.1399382    3.4732297    1.7039286
H    -0.1782828    4.4887380    1.9694218
H     0.3777878    2.9439325    2.6335521
H     1.0563011    3.5531001    1.1084309
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C	-1.5970519	3.4708862	-0.8554517
H	-1.9811625	4.4773815	-0.6480071
H	-0.7010308	3.5728072	-1.4770531
H	-2.3551998	2.9360792	-1.4364526

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7HmS- Energy = -1599.802233431

W	0.3841347	3.1192575	-0.1352590
Si	-0.4058853	-2.3004080	0.0920609
P	0.8220057	0.5992533	0.1051727
O	3.0612993	3.2910470	-1.9078741
O	2.1703257	3.4716420	2.5158208
O	-1.3062655	2.4247163	-2.7755191
O	-2.2184084	2.6403190	1.6859619
O	-0.1751122	6.2468166	-0.3972530
F	1.7519405	0.1400183	-1.1794254
C	1.2359354	-2.9522463	-0.5578045
C	-0.5084178	-2.5595812	1.9530768
C	2.0938188	3.2409083	-1.2716490
C	1.5225804	3.3594649	1.5628515
C	-1.8163700	-3.2340593	-0.7529841
C	-0.7001858	2.6923764	-1.8221625
C	-1.2813109	2.8284616	1.0267219
C	0.0311520	5.1020169	-0.2979345
H	1.3223711	-4.0307598	-0.3733530
H	1.3349795	-2.7814926	-1.6360681
H	2.0685953	-2.4447664	-0.0600723
H	0.2897771	-1.9891271	2.4394501
H	-0.3987468	-3.6193905	2.2155587
H	-1.7611172	-4.3090194	-0.5377705
H	-1.4697739	-2.2111507	2.3508463
H	-1.7773864	-3.1079677	-1.8422046
H	-2.7937702	-2.8732505	-0.4091527
O	1.4978805	0.0855665	1.3548208
C	-0.6243794	-0.4561368	-0.2941612
H	-0.8814716	-0.2974372	-1.3497113
H	-1.4681946	-0.0750713	0.2980165

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7H Energy = -2009.065211705

W	1.2620723	1.4323703	-2.7804864
P	-0.4126537	0.8743925	-1.0165124
O	-1.7784468	0.0817116	-1.4038911
H	-2.0705831	0.2617005	-2.3142296
F	-1.0562347	2.2726757	-0.5003477
O	-0.9213869	3.4028272	-4.0853823
O	0.2573326	-0.9399036	-4.7057159
O	2.2182978	3.8100714	-0.8358196
O	3.4180445	2.3027267	-4.9727866
O	3.4259783	-0.4826977	-1.3750935
Si	-0.7478025	0.7278979	2.0973838
Si	-0.0328839	-1.8973921	0.3058601
C	-1.7135812	-2.5510809	0.8342832
C	-2.6167621	0.8320893	1.9422646
C	-0.1388158	2.6919836	-3.6198596
C	-0.2930846	-0.3634832	3.5633985
C	0.0477244	0.0227992	0.4891215
C	0.0042693	2.4205573	2.4321379
C	0.2710797	-2.4860494	-1.4564381
C	0.6192356	-0.0946479	-4.0058902
C	1.3536235	-2.5955397	1.3681059
C	1.8775634	2.9590926	-1.5380263
C	2.6377589	1.9827839	-4.1794631
C	2.6457277	0.1966850	-1.8917433
H	-1.7319532	-3.6399419	0.7002556
H	-1.9488487	-2.3419892	1.8823384
H	-2.5056071	-2.1211883	0.2119569
H	-2.9183753	1.5082242	1.1366993
H	-3.0374092	1.2130708	2.8812697
H	-0.6878994	-1.3813748	3.4925968
H	-3.0641035	-0.1478793	1.7481845
H	-0.7126386	0.0921526	4.4697513
H	-0.5206279	-2.1752905	-2.1432231
H	-0.3338702	2.7898201	3.4084415
H	-0.2725148	3.1584722	1.6742956
H	0.2881018	-3.5838457	-1.4435295
H	0.7927812	-0.4242926	3.6973479
H	1.2404656	-2.3621078	2.4302728
H	1.1217830	0.2413734	0.5987010
H	1.3800284	-3.6872956	1.2637386
H	1.0990111	2.3587050	2.4633295
H	1.2312535	-2.1513145	-1.8593626
H	2.3239505	-2.2068682	1.0360661

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7- Energy = -2008.600899941

W	0.1474755	3.3964973	-0.1848825
Si	-0.1842520	-1.6815921	-1.4829087
Si	-0.0606190	-0.9416872	1.6487990
P	1.0631796	1.0009318	-0.4188365
O	2.3651336	0.5915106	0.2285177
O	2.7147180	4.2331083	-1.9333836
O	1.9100996	3.6924551	2.4873314
O	-1.4991657	2.7956957	-2.8773325
O	-2.3985268	2.3774442	1.4844173
O	-0.8772113	6.4092130	-0.0301841
F	1.3121228	0.8530052	-2.0531276
C	1.5495229	-2.3241879	-1.8399083
C	1.2299235	-2.3047351	1.8116156
C	0.4068788	0.4066183	2.8813321
C	-0.9776349	-1.0104707	-3.0580444
C	1.7893715	3.9382692	-1.3014614
C	-0.1844238	-0.3243945	-0.1497412
C	-1.2551215	-3.1530967	-0.9619826
C	1.2663634	3.5902190	1.5295807
C	-1.7631206	-1.5727300	2.1755774
C	-0.9059875	3.0273192	-1.9081520
C	-1.4690393	2.7470712	0.8935257
C	-0.5038009	5.3040801	-0.0801552
H	1.3326430	-2.6006287	2.8635145
H	0.9819944	-3.2016458	1.2341227
H	1.9923381	-2.7931256	-0.9550296
H	2.1970982	-1.9262941	1.4629146
H	1.5103944	-3.0771589	-2.6378374
H	2.2122174	-1.5143524	-2.1578432
H	1.3981977	0.8116893	2.6625060
H	-1.0503838	-1.8030381	-3.8141158
H	-0.4049964	-0.1799303	-3.4790456
H	0.4229005	-0.0310030	3.8888386
H	-1.2743300	-3.8837637	-1.7817752
H	-0.8772519	-3.6650330	-0.0707798
H	-1.7378682	-1.8873725	3.2269576
H	-0.3091680	1.2340923	2.8921545
H	-1.9939792	-0.6504608	-2.8545276
H	-2.1079761	-2.4220827	1.5782162
H	-1.1690273	0.1610321	-0.2406872
H	-2.2898849	-2.8488470	-0.7650853
H	-2.5088036	-0.7726214	2.0869058

42

7 Energy = -2008.420936424

W	0.3156157	3.4073161	-0.0939662
Si	-0.2622408	-1.7722966	-1.5140023
Si	-0.0513875	-0.9543411	1.6439651
P	0.8792098	0.9746994	-0.5649694
O	2.2186186	0.8749672	0.1388929
O	3.0396331	4.3189279	-1.5621962
O	1.6324614	3.9256665	2.8151527

O	-1.0052998	3.1077096	-3.0153572
O	-2.3463385	2.3042961	1.3169407
O	-1.0604092	6.2797233	-0.1836561
F	1.1421892	0.8174608	-2.1542398
C	1.4837669	-2.3450292	-1.9018398
C	1.2981985	-2.2563868	1.7499843
C	0.4117068	0.4349096	2.8258337
C	-1.1314366	-1.1216219	-3.0503980
C	2.0703194	4.0001517	-1.0317273
C	-0.2563433	-0.3722085	-0.1848093
C	-1.2758102	-3.2308075	-0.8877341
C	1.1725012	3.7145316	1.7835704
C	-1.7237039	-1.6139715	2.1993786
C	-0.5319932	3.2044484	-1.9718150
C	-1.3843263	2.7074063	0.8231350
C	-0.5371379	5.2511924	-0.1309535
H	1.4362934	-2.5503909	2.7978002
H	1.0704685	-3.1610173	1.1777294
H	1.9879591	-2.7428256	-1.0154249
H	2.2489451	-1.8496486	1.3873140
H	1.4411076	-3.1472768	-2.6491911
H	2.0990349	-1.5377022	-2.3103355
H	1.3780359	0.8776108	2.5720893
H	-1.2542808	-1.9338248	-3.7777256
H	-0.5770591	-0.3131182	-3.5346698
H	0.4883853	0.0049086	3.8332308
H	-1.3134424	-3.9824748	-1.6869770
H	-0.8475639	-3.7106561	-0.0025414
H	-1.6684323	-1.8923663	3.2591856
H	-0.3410721	1.2276082	2.8706939
H	-2.1320578	-0.7486337	-2.7998073
H	-2.0528269	-2.4918602	1.6377468
H	-1.2616179	0.0725723	-0.2510338
H	-2.3065893	-2.9392191	-0.6582813
H	-2.4930806	-0.8384291	2.1010083

34

CPh_3 Energy = -733.4910462718

C	0.0000000	0.0000000	0.0000000
C	-0.7286857	1.2621206	0.0000000
C	-0.7286857	-1.2621206	0.0000000
C	-0.2144845	2.4072908	0.6529237
C	-0.2144845	-2.4072908	-0.6529237
C	-1.9775327	-1.3893945	0.6529237
C	-1.9775327	1.3893945	-0.6529237
C	-0.9130012	3.6094877	0.6554034
C	-0.9130012	-3.6094877	-0.6554034
C	1.4573713	0.0000000	0.0000000
C	-2.6694074	-2.5954261	0.6554034
C	-2.6694074	2.5954261	-0.6554034
C	-2.1444033	-3.7142154	0.0000000
C	-2.1444033	3.7142154	0.0000000
C	2.1920173	1.0178964	-0.6529237
C	2.1920173	-1.0178964	0.6529237
C	3.5824086	-1.0140616	0.6554034
C	3.5824086	1.0140616	-0.6554034
C	4.2888065	0.0000000	0.0000000
H	0.7312956	2.3328645	1.1810619
H	0.7312956	-2.3328645	-1.1810619
H	-2.3859677	-0.5331117	1.1810619
H	-2.3859677	0.5331117	-1.1810619
H	1.6546721	-1.7997528	1.1810619
H	1.6546721	1.7997528	-1.1810619
H	-0.5010088	4.4683135	1.1785065
H	-0.5010088	-4.4683135	-1.1785065
H	-3.6191686	-2.6680431	1.1785065
H	-3.6191686	2.6680431	-1.1785065
H	-2.6874960	4.6548797	0.0000000
H	-2.6874960	-4.6548797	0.0000000
H	4.1201774	-1.8002704	1.1785065
H	4.1201774	1.8002704	-1.1785065
H	5.3749921	0.0000000	0.0000000

34

CPh_3+ Energy = -733.3236327450

C	0.0004526	-0.0002639	0.0000421
C	-0.7212253	1.2378460	-0.1701043
C	-0.7213720	-1.2378155	0.1724051
C	-0.1892361	2.4554871	0.3237376
C	-0.1918586	-2.4557876	-0.3234131
C	-1.9715086	-1.2547784	0.8406351
C	-1.9735861	1.2554762	-0.8340486
C	-0.8934137	3.6395163	0.1696740
C	-0.8963068	-3.6393342	-0.1672530
C	1.4434993	-0.0004875	-0.0023082
C	-2.6542299	-2.4483034	1.0163240
C	-2.6562300	2.4493895	-1.0074620
C	-2.1228353	-3.6392132	0.5074914
C	-2.1221218	3.6401033	-0.5010145
C	2.1624095	0.9303996	-0.7937550
C	2.1648709	-0.9315600	0.7866452
C	3.5509818	-0.9178591	0.7917731
C	3.5485258	0.9170556	-0.8028239
C	4.2441687	-0.0002690	-0.0064680
H	0.7448582	2.4423246	0.8749288
H	0.7403640	-2.4432286	-0.8777902
H	-2.3596948	-0.3351264	1.2649235
H	-2.3636181	0.3360092	-1.2570574
H	1.6223024	-1.6147408	1.4311534
H	1.6177845	1.6132144	-1.4368892
H	-0.4956916	4.5631123	0.5770519
H	-0.5005339	-4.5631426	-0.5760364
H	-3.5953543	-2.4595437	1.5561036
H	-3.5995737	2.4610229	-1.5433505
H	-2.6651766	4.5714211	-0.6294485
H	-2.6664064	-4.5700876	0.6369560
H	4.0971523	-1.6122549	1.4216151
H	4.0927213	1.6114397	-1.4343829
H	5.3298824	-0.0000213	-0.0078541

14

$PhCH_2$ Energy = -271.0826274800

C	2.3234141	-0.1563782	0.0000000
C	-1.2040812	0.0785913	-1.2134115
C	0.1788362	-0.0134144	-1.2186078
C	0.9190479	-0.0627327	0.0000000
C	0.1788362	-0.0134144	1.2186078
C	-1.2040812	0.0785913	1.2134115
C	-1.9083706	0.1253956	0.0000000
H	2.8803185	-0.1938299	0.9313088
H	2.8803185	-0.1938299	-0.9313088
H	-1.7462783	0.1148585	-2.1544880
H	0.7203521	-0.0492050	-2.1608534
H	0.7203521	-0.0492050	2.1608534
H	-1.7462783	0.1148585	2.1544880
H	-2.9919983	0.1978672	0.0000000

15

$PhCH_3$ Energy = -271.7322720111

C	2.2326809	-0.0029986	0.0000000
H	2.6100031	1.0277623	0.0000000
C	-1.3928032	0.0029447	-1.2066979
C	0.0031787	-0.0136599	-1.2021841
C	0.7230344	-0.0183818	0.0000000
C	0.0031787	-0.0136599	1.2021841
C	-1.3928032	0.0029447	1.2066979
C	-2.0968501	0.0127151	0.0000000
H	2.6336484	-0.4998771	0.8888229

H 2.6336484 -0.4998771 -0.8888229
H -1.9300969 0.0043613 -2.1513804
H 0.5434870 -0.0257715 -2.1464944
H 0.5434870 -0.0257715 2.1464944
H -1.9300969 0.0043613 2.1513804
H -3.1833085 0.0230609 0.0000000

30
TEMPH$_2$+ Energy = -409.8689320610
N 0.9373346 0.1605298 0.0000000
H 1.7420319 -0.4760162 0.0000000
H 1.3332529 1.1072367 0.0000000
C -1.1047550 0.8083578 1.2567865
C 0.1955159 0.0005834 1.3516470
C -1.9214448 0.4969618 0.0000000
C -0.0402598 -1.4817774 1.6431454
C 0.1955159 0.0005834 -1.3516470
C -0.0402598 -1.4817774 -1.6431454
C 1.1487817 0.5957925 -2.3917870
C -1.1047550 0.8083578 -1.2567865
C 1.1487817 0.5957925 2.3917870
H -0.8197339 -1.9190692 1.0193342
H -0.8594688 1.8784975 1.2728019
H -1.6849803 0.5996144 2.1600969
H 0.8800145 -2.0623081 -1.5191628
H -2.2501543 -0.5484555 0.0000000
H 1.3666687 1.6468543 -2.1724664
H 2.0897425 0.0366811 -2.4347297
H -0.8197339 -1.9190692 -1.0193342
H -2.8285977 1.1082054 0.0000000
H 0.8800145 -2.0623081 1.5191628
H -0.8594688 1.8784975 -1.2728019
H -0.3563254 -1.5728771 2.6859917
H 1.3666687 1.6468543 2.1724664
H -0.3563254 -1.5728771 -2.6859917
H 0.6785885 0.5454197 -3.3772151
H 0.6785885 0.5454197 3.3772151
H -1.6849803 0.5996144 -2.1600969
H 2.0897425 0.0366811 2.4347297

30
TEMPOH Energy = -484.6278629345
N 0.8683398 0.3024933 0.0000000
C -1.1509630 0.8387399 1.2497524
C 0.1659132 0.0383992 1.2897433
C -1.9824767 0.5494297 0.0000000
C -0.0995194 -1.4479834 1.6073515
C 0.1659132 0.0383992 -1.2897433
C -0.0995194 -1.4479834 -1.6073515
C 1.0647163 0.6199456 -2.3929352
C -1.1509630 0.8387399 -1.2497524
C 1.0647163 0.6199456 2.3929352
H -0.9277142 -1.8598258 1.0274545
H -0.9099483 1.9091190 1.2836734
H -1.7149662 0.6055665 2.1606395
H 0.7968590 -2.0418073 -1.4099195
H -2.3198956 -0.4944789 0.0000000
H 1.3457360 1.6482803 -2.1417535
H 1.9748795 0.0242996 -2.5082594
H -0.9277142 -1.8598258 -1.0274545
H -2.8868057 1.1692356 0.0000000
H 0.7968590 -2.0418073 1.4099195
H -0.9099483 1.9091190 -1.2836734
H -0.3536191 -1.5481788 2.6686218
H 1.3457360 1.6482803 2.1417535
H -0.3536191 -1.5481788 -2.6686218
H 0.5291920 0.6201107 -3.3486395
H 0.5291920 0.6201107 3.3486395
H -1.7149662 0.6055665 -2.1606395
H 1.9748795 0.0242996 2.5082594
O 2.0931289 -0.5096285 0.0000000
H 2.7865777 0.1696175 0.0000000

29
TEMPO- Energy = -484.0919124136
N 0.8799050 0.5735637 -0.0076164
C -1.2587336 0.5182788 1.2439643
C 0.2300540 0.1306509 1.2683723
C -1.9817682 -0.0139085 0.0075258
C 0.4239163 -1.3698652 1.5770861
C 0.2202509 0.1124720 -1.2719487
C 0.4108449 -1.3927053 -1.5593315
C 0.9086713 0.9022932 -2.3948451
C -1.2679773 0.5014167 -1.2413006
C 0.9274839 0.9371114 2.3734968
O 2.2374105 0.1454257 -0.0098544
H -1.3263374 1.6160900 1.2445537
H -1.7357087 0.1610525 2.1673348
H -1.9876878 -1.1118493 0.0149668
H -3.0327092 0.3052698 0.0091857
H -0.3100469 -2.0032594 1.0699311
H 1.4313324 -1.6267513 1.2275433
H 0.3496488 -1.5616219 2.6551464
H 1.4209583 -1.6450327 -1.2141840
H -0.3191905 -2.0176687 -1.0363040
H 0.3274676 -1.6010862 -2.6336375
H 0.8013431 1.9757930 -2.2016988
H 1.9735219 0.6548318 -2.4020283
H 0.4629224 0.6652453 -3.3698340
H -1.3343719 1.5990860 -1.2553510
H -1.7522988 0.1328757 -2.1563647
H 0.8226858 2.0070061 2.1615942
H 0.4868368 0.7188416 3.3551464
H 1.9915762 0.6864446 2.3784514

29
TEMPO Energy = -484.0199169843
N 0.9404027 -0.1237507 0.0000000
C -0.9217772 0.9764852 1.2414248
C 0.2437423 -0.0223963 1.3309191
C -1.7882260 0.7783737 0.0000000
C -0.2455350 -1.4234679 1.7464627
C 0.2437423 -0.0223963 -1.3309191
C -0.2455350 -1.4234679 -1.7464627
C 1.2777601 0.4804312 -2.3465278
C -0.9217772 0.9764852 -1.2414248
C 1.2777601 0.4804312 2.3465278
O 2.0689367 -0.7479501 0.0000000
H -0.5122153 1.9952907 1.2272882
H -1.5139009 0.8788519 2.1583952
H -2.2451356 -0.2187836 0.0000000
H -2.6109307 1.5018489 0.0000000
H -1.0838014 -1.7633473 1.1328670
H 0.5742498 -2.1412515 1.6533363
H -0.5751787 -1.3965102 2.7902466
H 0.5742498 -2.1412515 -1.6533363
H -1.0838014 -1.7633473 -1.1328670
H -0.5751787 -1.3965102 -2.7902466
H 1.6891081 1.4435854 -2.0279619
H 2.0960055 -0.2342538 -2.4549917
H 0.7886410 0.6124826 -3.3171554
H -0.5122153 1.9952907 -1.2272882
H -1.5139009 0.8788519 -2.1583952
H 1.6891081 1.4435854 2.0279619
H 0.7886410 0.6124826 3.3171554
H 2.0960055 -0.2342538 2.4549917

29

TEMPO+ Energy = -483.8301174894

N	0.8796876	0.4263857	-0.0065854
C	-1.2515401	0.5132242	1.2503021
C	0.2432049	0.1054984	1.3427946
C	-1.9527266	-0.0218493	0.0079332
C	0.4114530	-1.4109780	1.6063621
C	0.2324912	0.0859107	-1.3460435
C	0.3984967	-1.4342509	-1.5890229
C	0.9633556	0.8709226	-2.4276128
C	-1.2614329	0.4953336	-1.2474853
C	0.9824878	0.9062455	2.4069622
O	1.9215405	1.0216338	-0.0150688
H	-1.3069835	1.6072767	1.2699105
H	-1.7168328	0.1426253	2.1687705
H	-1.9906187	-1.1159526	0.0159017
H	-2.9913864	0.3238315	0.0096083
H	-0.2648105	-2.0217533	1.0119689
H	1.4433220	-1.7278410	1.4398806
H	0.1703520	-1.5548465	2.6627071
H	1.4315985	-1.7489459	-1.4261351
H	-0.2731590	-2.0362597	-0.9806096
H	0.1489901	-1.5932238	-2.6412321
H	0.9574179	1.9428917	-2.2149180
H	1.9961777	0.5355778	-2.5454166
H	0.4311946	0.6954595	-3.3658641
H	-1.3168677	1.5890436	-1.2823423
H	-1.7341376	0.1118438	-2.1568401
H	0.9741481	1.9750796	2.1790065
H	0.4581384	0.7439843	3.3519642
H	2.0164392	0.5731329	2.5211039

28

TEMP- Energy = -408.8380337409

N	0.9616228	0.5461016	0.0000000
C	-1.1938458	0.4868911	1.2666659
C	0.3240445	0.1482019	1.2328548
C	-1.9051469	-0.0059525	0.0000000
C	0.4870202	-1.3633473	1.6240670
C	0.3240445	0.1482019	-1.2328548
C	0.4870202	-1.3633473	-1.6240670
C	1.0245349	0.9550203	-2.3407403
C	-1.1938458	0.4868911	-1.2666659
C	1.0245349	0.9550203	2.3407403
H	-1.2995612	1.5784911	1.3471551
H	-1.6758035	0.0526533	2.1584062
H	-1.9237699	-1.1057364	0.0000000
H	-2.9561784	0.3169605	0.0000000
H	-0.1701544	-2.0128125	1.0365980
H	1.5218565	-1.6646573	1.4235312
H	0.2604947	-1.5398312	2.6877980
H	1.5218565	-1.6646573	-1.4235312
H	-0.1701544	-2.0128125	-1.0365980
H	0.2604947	-1.5398312	-2.6877980
H	0.9800019	2.0183199	-2.0771849
H	2.0827877	0.6659917	-2.3881582
H	0.5707361	0.7971826	-3.3301935
H	-1.2995612	1.5784911	-1.3471551
H	-1.6758035	0.0526533	-2.1584062
H	0.9800019	2.0183199	2.0771849
H	0.5707361	0.7971826	3.3301935
H	2.0827877	0.6659917	2.3881582

28

TEMP Energy = -408.7570106420

N	0.5114827	0.8176486	0.4208114
C	0.5945406	-1.6877581	0.0215153
C	1.2650138	-0.3042732	-0.1408710
C	-0.8943570	-1.6519113	-0.3167126
C	1.5059928	-0.0009008	-1.6439118
C	-0.9516319	0.7851594	0.4365426
C	-1.4491380	1.4517677	-0.8739174
C	-1.3874981	1.6696565	1.6183143
C	-1.5719916	-0.6229208	0.5857510
C	2.6292730	-0.3043092	0.5716778
H	0.5919294	-0.1131901	-2.2317877
H	0.7113355	-2.0115814	1.0649008
H	1.1310021	-2.4131964	-0.6018445
H	-0.9281454	2.3995549	-1.0375777
H	-1.0439909	-1.3962791	-1.3734845
H	-1.0067366	1.2586848	2.5591765
H	-0.9949858	2.6845758	1.4984508
H	-1.2861172	0.8095759	-1.7426161
H	-1.3414917	-2.6412418	-0.1667468
H	1.8784522	1.0200025	-1.7688466
H	-1.4617210	-0.9435420	1.6308388
H	2.2556123	-0.7006287	-2.0297201
H	2.4948200	-0.4623029	1.6469181
H	-2.5230162	1.6492924	-0.7841064
H	3.2639147	-1.1066268	0.1779150
H	-2.4811696	1.7163179	1.6751913
H	3.1360414	0.6544398	0.4221088
H	-2.6474195	-0.5560136	0.3820308

12

THFmH Energy = -231.9373294588

O	-1.5260503	-0.2847670	0.1020836
C	0.7012197	0.0928374	0.8767523
C	0.6993697	-0.0841138	-0.6611464
C	-0.7513941	0.2291042	-1.0222283
C	-0.7327493	-0.1809536	1.2345245
H	1.3992304	-0.5877541	1.3776538
H	0.9345186	-1.1203444	-0.9236863
H	1.0006776	1.1165361	1.1459847
H	1.4057145	0.5759682	-1.1705447
H	-0.9300665	1.3089568	-1.1025670
H	-1.1198264	-0.2728783	-1.9183513
H	-1.0806439	-0.7925914	2.0615251

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THF Energy = -232.5923565762

O	-1.4042011	-0.4952846	0.0000000
C	0.7948738	-0.0686383	0.7775057
C	0.7948738	-0.0686383	-0.7775057
C	-0.6977077	0.0311156	-1.1400844
C	-0.6977077	0.0311156	1.1400844
H	1.2238864	-0.9972744	1.1629451
H	1.2238864	-0.9972744	-1.1629451
H	1.3642089	0.7661878	1.1951692
H	1.3642089	0.7661878	-1.1951692
H	-0.9940700	1.0790849	-1.3026705
H	-0.9940700	1.0790849	1.3026705
H	-0.9890908	-0.5628335	-2.0090793
H	-0.9890908	-0.5628335	2.0090793