Electronic Supplementary Information (ESI)

Formation and properties of phosphaquinomethane tungsten(0) complexes – isolation and conversion of primary radical coupling products

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Abstract: The rational approach to phosphaquinomethane metal(0) com-plexes, based on dearomatization of the phenylene unit in $[W(CO)_5](R)P(Cl)\text{-}C_6H_4\text{-}CPh_2$, is described, including theoretical stu-dies on mechanisms and structures. Furthermore, the first phos-phaquinone tungsten complex with reversible redox properties is reported thus illustrating the beneficial stabilization of ligation.

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Experimental Procedures

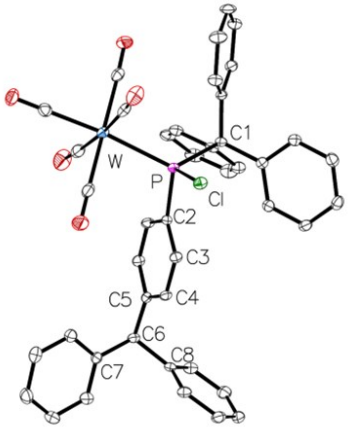
All reactions were carried out under an inert gas atmosphere using purified and dried argon and standard Schlenk techniques. Tetrahydrofuran, diethyl ether, and *n*-pentane were dried over sodium wire/benzophenone, CH_2Cl_2 over CaH_2 and further purified by subsequent distillation. All NMR spectra were recorded on a Bruker AVI-300 (300.1 MHz for ^{1}H, 75.5 MHz for ^{13}C and 121.5 MHz for ^{31}P), Bruker AVI-400 (400.1 MHz for ^{1}H, 100.6 MHz for ^{13}C and 162.0 MHz for ^{31}P), Bruker AV III HD Prodigy 500 (500.2 MHz for ^{1}H, 125.8 MHz for ^{13}C and 202.5 MHz for ^{31}P), and Bruker AV III HD Cryo 700 (700.4 MHz for ^{1}H, 176.1 MHz for ^{13}C and 283.5 MHz for ^{31}P) spectrometer at 25 °C. 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, respectively, and ^{31}P spectra were referenced to 85% H_3PO_4 as an external standard. Melting points were determined in one-side melted off capillaries using a Büchi Type S or a Carl Roth Type MPM-2 apparatus, they 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 or a MAT 90 Thermo Finnigan sector instrument equipped with a LIFDI ion source. IR spectra of all compounds were recorded on a Thermo Nicolet 380 FT-IR spectrometer with an attenuated total reflection (ATR) attachment or a Bruker Alpha Diamond ATR FTIR spectrometer. The molecular structures in the single crystal were solved by direct methods refined by full-matrix least-squares technique in anisotropic approximation for non-hydrogen atoms using SHELXS97 and SHELXL9723 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 (CCDC) as CCDC nos. 2023915, which can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif.

*Synthesis of complex **2**.* To a THF solution of the dichlorophosphane tungsten(0) complex (545 mg, 0.814 mmol), ^{t}butyl lithium (0.896 mmol, 1.6 mol/L) were slowly added at -78 °C. After 15 min $[Ph_3C]BF_4$ (294 mg, 0.896 mmol) of was slowly added in solid form at -78 °C. The reaction solution was stirred and warmed up slowly to -50 °C and then kept at -50°C for another 30 min. The solvent was removed in vacuo (10^{-2}-10^{-3} mbar) between -50 and -55 °C and a white-grey powder was obtained. The product was extracted with a mixture of pentane/toluene (10:2) and a white solid was obtained.

2: Yield: 300 mg (42%); m. p. = 159-161 °C; ^{1}H NMR (300.1 MHz, C_6D_6, r.t.) δ / ppm = 4.7 (m, $^2J_{P,H}$ = 29.1 Hz, P-C*H*, 1H), 5.0 (m, P-CH-C*H*, 1H), 6.1 (m, P-CH-C*H*, 1H), 6.7 (m, P-CH-CH=C*H*, 1H), 7.0 (m, P-CH-CH=C*H*, 1H), 6.8-7.8 (m, Ph, 25H); ^{13}C{^{1}H} NMR (100.6 MHz, C_6D_6, r.t.): δ / ppm = 54.9 (d, $^1J_{P,C}$ = 1.2 Hz, P-*C*H), 70.4 (d, $^1J_{P,C}$ = 12.2 Hz, *C*Ph_3), 124.4 (s, P-CH-CH), 126.2 (d, $^2J_{P,C}$ = 3.3 Hz, P-CH-CH), 127-131 (s, Ph), 132.1 (d, $^2J_{P,C}$ = 12.3 Hz, P-CH-CH=CH), 132.5 (d, $^2J_{P,C}$ = 11.3 Hz, P-CH-CH=CH), 140.1 (d, $^2J_{P,C}$ = 4.2 Hz, *ipso*-Ph), 141.3 (d, $^2J_{P,C}$ = 5.3 Hz, *ipso*-Ph), 141.4 (d, $^2J_{P,C}$ = 5.2 Hz, *ipso*-Ph), 141.9 (s, *ipso*-Ph), 142.1 (s, P-C=C-C=C), 142.3 (s, *ipso*-Ph), 143.3 (d, $^xJ_{P,C}$ = 1.1, Hz, P-C=C-C=C), 196.8 (d_{Sat}, $^2J_{P,C}$ = 6.0 Hz, $^1J_{W,C}$ = 128.2, *cis*-CO), 198.5 (d, $^2J_{P,C}$ = 37.2 Hz, *trans*-CO); ^{31}P (121.5 MHz, C_6D_6, r.t.) δ / ppm = 147.8 (s_{sat}, $^2J_{P,H}$ = 29.1 Hz, $^1J_{W,P}$ = 275.8 Hz; MS (Lifdi): $[M\text{-}CHPh_3]^+$ (30), $[CHPh_3]^+$ (100); IR (ATR Diamond) $\tilde{\nu}$ / cm^{-1} = *ν*(CO): 3053 (b, *ν*-CH_2), 2070 (b, *ν*-CO), 2060 (s, *ν*-CO), 1984 (s, *ν*-CO), 1918 (s, *ν*-CO). Elemental analysis for $C_{43}H_{30}ClO_5PW$ (876.97 g/mol): calc: C 59.37 %, H 3.59 %; exp: C 58.89 %, H 3.45 %.

*Synthesis of complex **3**.* To a solution of the dichlorophosphane tungsten(0) complex (545 mg, 0.815 mmol) in THF (5 mL), 0.53 mL (0.901 mmol, 1.7 mol/L) of ^{t}butyllithium was slowly added at -85 °C (to form complex **1**) under continuous stirring. After stirring for 15 min, $[Ph_3C]BF_4$ (269 mg, 0.815 mmol) was added at -85 °C. The reaction mixture was stirred for 40 min while keeping the temperature below -50 °C, before removing the THF (-50 °C, 10^{-2}-10^{-3} mbar) and extracting the product with toluene. The solution was cooled down to -30 °C before adding Et_3N (0.3 mL, 4.1 mmol). The reaction mixture was allowed to warm up to ambient temperature overnight. The toluene was evaporated and the remaining grey solid was filtered through SiO_2 (15 cm SiO_2, Ø 3 cm, r.t., under air, 500 mL Et_2O) with Et_2O. The solvent was evaporated and the remaining beige solid was dried in vacuo (10^{-2} mbar) for 3 h.

3: Yield: 310 mg (43 %); m.p. 150 °C; ^{1}H NMR (500.1 MHz, $CDCl_3$, r.t.) δ / ppm = 5.51 (s, C*H*Ph_2), 6.70-6.76 (m, CPh_3), 6.93-6.94 (m, P-Ar), 7.06-7.12 (m, CPh_3), 7.17-7.24 (m, CPh_3), 7.25-7.29 (m, $CHPh_2$), 7.30-7.34 (m, CPh_3), 7.37-7.44 (m, CPh_3,), 7.58-7.63 (m, CPh_3), 7.63-7.68 (m, CPh_3). ^{13}C{^{1}H} NMR (176.1 MHz, $CDCl_3$, r.t.) δ / ppm = 56.4 (*C*HPh_2), 70.3 (d, $^1J_{P,C}$ = 4.5 Hz, *C*Ph_3), 126.7 (d, $^XJ_{P,C}$ = 2.0 Hz, CPh_3), 127.4 (CPh_3), 127.7 (CPh_3), 128.3 (CPh_3), 128.6 ($CHPh_2$), 128.7 (CPh_3), 128.9 (d, $^XJ_{P,C}$ = 9.2 Hz, P-Ar), 129.5 ($CHPh_2$), 131.0 (d, $^XJ_{P,C}$ = 2.2 Hz, CPh_3), 131.2 (d, $^XJ_{P,C}$ = 11.7 Hz, P-Ar), 131.8 (d, $^XJ_{P,C}$ = 7.4 Hz, CPh_3), 136.1 (d, $^1J_{P,C}$ = 17.2 Hz, P-C), 139.2 (d, $^2J_{P,C}$ = 5.9 Hz, *ipso*-C, CPh_3), 139.8 (d, $^2J_{P,C}$ = 5.6 Hz, *ipso*-C, CPh_3), 143.2 (*ipso*-C, $CHPh_2$), 143.3 (*ipso*-C, $CHPh_2$), 143.6 (d, $^2J_{P,C}$ = 8.9 Hz, *ipso*-C, CPh_3), 146.7 (d, $^4J_{P,C}$ = 1.4 Hz, P-Ar), 196.9 (d_{sat}, $^2J_{P,C}$ = 6.3 Hz, $^1J_{W,C}$ = 128.2 Hz, *cis*-CO), 199.3 (d_{sat}, $^2J_{P,C}$ = 34.5 Hz, $^1J_{W,C}$ = 143.7 Hz, *trans*-CO). ^{31}P{^{1}H} NMR (202.5 MHz, $CDCl_3$, r.t.) δ / ppm = 118.8 (s_{sat}, $^1J_{W,P}$ = 271.0 Hz). MS (EI, 70 eV, ^{184}W) m/z (%) = 764.1 (0.007) $[M\text{-}Ph\text{-}Cl]^+$, 680.1 (0.02) $[M\text{-}Ph\text{-}Cl\text{-}3CO]^+$, 633.0 (0.04) $[M\text{-}CPh_3]^+$, 492.0 (0.2) $[M\text{-}Cl\text{-}Ph\text{-}CPh_3\text{-}CO]^+$, 458.0 (0.1) $[M\text{-}Cl\text{-}CPh_3\text{-}5CO]^+$, 243.1 (100) $[CPh_3]^+$. IR (ATR Diamond) $\tilde{\nu}$ / cm^{-1} = *ν*(CO): 2072.7 (s), 1998.2 (m), 1907.7 (vs). Elemental analysis for $C_{43}H_{30}ClO_5PW$ (876.97 g/mol): calc: C 58.89 %, H 4.25 %; exp: C 59.70 %, H 3.72 %.



*Crystal Data for **3**:* Suitable single crystals of **3** were obtained from a concentrated diethylether solution at 4 °C. Data were collected with a Bruker D8-Venture diffractometer equipped with a low-temperature device at 100.0 K by using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structure was solved by Patterson methods (SHELXS-97) and refined by full-matrix least squares on F2 (SHELXL-97):$C_{47}H_{40}ClO_6PW$, M_r = 951.06, crystal dimensions 0.16 × 0.14 × 0.1 mm^3, triclinic, space group P-1, Z = 2, a = 10.9641(8) Å, b = 13.1791(8) Å, c = 14.2135(10) Å, α = 80.151(3)°, β = 84.789(3)°, γ = 82.795(3)°, V = 2002.5(2) Å^3, ρ_{calc} = 1.577 g cm^{-3}, μ = 3.041 mm^{-1}, transmission factors (min/max) 0.5693/0.7459, empirical absorption correction, 2θmax = 56°, no. of unique data 9658, R_{int} = 0.0320, R_1 (for I >2σ(I)) = 0.0186, wR_2 (for all data) = 0.0445, final R_1 = 0.0217, goodness of fit 1.075, ΔF (max/min) = 1.15 /−0.54 e Å^{-3}. CCDC 2023915.

*Synthesis of complex **4**.* A THF solution (1 mL) of KHMDS (35.8 mg, 0.1796 mmol) was added drop wise to a THF solution (2 mL) of complex **2** (157.5 mg, 0.1796 mmol) at -40°C in the glove box. The colorless solution turned immediately to deep blue-violet color. After 40 minutes stirring the solvent was exchanged by diethyl ether and the reaction mixture was filtered over silanized SiO_2. After evaporation of the solvent in vacuo (10^{-2} mbar) a dark blue solid was obtained.

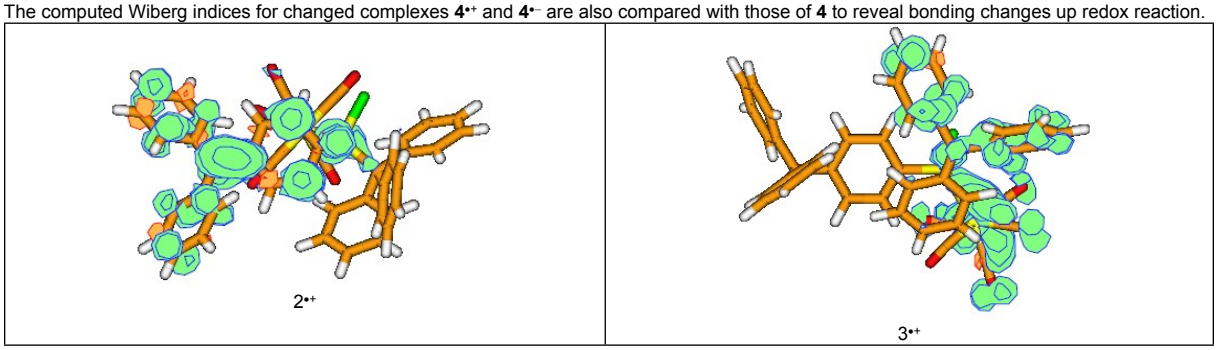
4: Yield: 110 mmg (73 %); m. p. = 146-148 °C, ^{1}H NMR (300.1 MHz, $CDCl_3$, r.t.): δ / ppm = 6.0 (dd, $^3J_{P,H}$ = 3.5 Hz, $^3J_{H,H}$ = 10.2 Hz, P=C-C*H*, 2H), 6.5 (d, $^3J_{H,H}$ = 10.2 Hz, P=C-CH=C*H*, 2H), 6.9-7.6 (m, Ph, 25H); ^{13}C{^{1}H} NMR (100.6 MHz, $CDCl_3$, r.t.): δ / ppm = 69.7 (s, CPh_3), 126-134 (Ph), 128.4 (s, P=C-C=C), 129.0 (s, P=C-C=C), 130.2 (s, P=C-C=C), 137.5 (s, P=C-C=C), 141.8 (d, $^4J_{P,C}$ = 17.8 Hz, P=C-C=C-C=C), 144.6 (d, $^5J_{P,C}$ = 3.9 Hz, P=C-C=C-C=C), 166.8 (d, $^1J_{P,C}$ = 36.2 Hz, P=C), 195.8 (d_{Sat}, $^2J_{P,C}$ = 13.2 Hz, $^1J_{W,C}$ = 126.9, *cis*-CO), 199.8 (d, $^2J_{P,C}$ = 34.4 Hz, $^1J_{W,C}$ = 145.7, *trans*-CO); ^{31}P (121.5 MHz, $CDCl_3$, r.t.) δ / ppm = 212.9 ppm (s_{sat}, $^1J_{W,P}$ = 270.3 Hz); IR (ATR Diamond) $\tilde{\nu}$ / cm^{-1} = *ν*(CO): 2962 (b, *ν*-CH_2), 2065 (b, *ν*-CO), 1985 (s, *ν*-CO), 1913 (b, *ν*-CO); UV-vis (Et_2O): λ_{max} (abs., ε / L mol^{-1} cm^{-1}) = 238.0 (0.682, 56833); 336.0 (0.114, 9500); 563 (0.092, 7667); Elemental analysis for $C_{42}H_{30}O_5PW$ (840.5 g/mol): calc: C 61.45 %, H 3.48 %, exp: C 62.8 %, H 4.64 %.

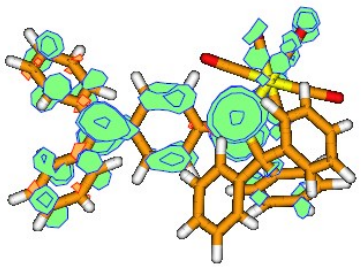
Computational Details: The TURBOMOLE V7.0 suite of programs[1] was used for all DFT calculations. All structures are fully optimized at the TPSS-D3/def2-TZVP + COSMO(THF) level of theory, which combines the TPSS meta-GGA density functional[2] with the BJ-damped DFT-D3 dispersion correction[3],[4] and the large def2-TZVP AO basis set,[5],[6] together with the COSMO (for THF solvent: dielectric constant ε_r = 7.58, R_{sol} = 3.18 Å) solvation model[7]. The density-fitting RI-J approach[8],[9] is used to accelerate the geometry optimization and harmonic frequency calculations. Vibrational frequency analysis is used to identify the nature of located stationary points and to provide thermal and free-energy corrections according to the modified ideal gas-rigid rotor-harmonic oscillator model.[10] The structures are characterized as true minima (with no imaginary frequency) or transition states (with only one imaginary frequency). To get more insights into the electronic structures, the Wiberg bond indices and the spin densities for open-shell species are also computed at the TPSS-D3/def2-TZVP + COSMO(THF) level, according to the Wiberg and the Mulliken population analysis, respectively.

Better free energies in THF solution are obtained from the sum of TPSS-D3/def2-QZVP single-point energies,[6] COSMO-RS[11] solvation free energies in THF (using the BP_TZVP_C30_1301.ctd parameter and the default G_{solv} = molar option), and TPSS-D3/def2-TZVP thermal corrections at 298.15 K related to ideal gas under 1 atm. Note that the computed G_{sol} values are added by +1.90 kcal/mol to convert into normal standard state of 1 mol/L concentration for all species in solution; for THF molecule, an additional free energy correction of 1.49 kcal/mol is added to account for its high concentration as solvent. For the computation of reduction potentials in acetonitrile instead of THF, COSMO-RS solvation free-energies in acetonitrile are also computed using the same BP_TZVP_C30_1301.ctd parameter. In our discussion, the final TPSS-D3/def2-QZVP + COSMO-RS(THF) free energies (in kcal/mol) are used unless specified otherwise.

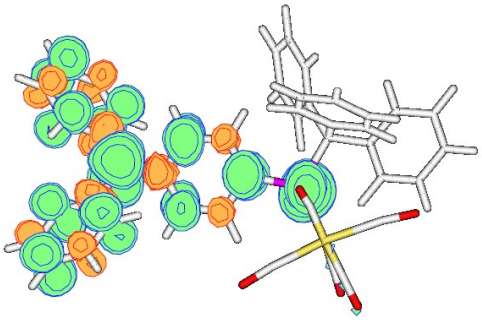
To analyze the UV/vis absorption spectra of the novel phosphaquinomethane complex **4**, TD-DFT calculations[12] for the lowest 20 singlet excited states are performed using hybrid PBE0 functional[13] together with the def2-TZVPD basis set[14] and the above TPSS-D3/def2-TZVP + COSMO(THF) optimized geometries. Single-point PBE0/def2-TZVP calculations are used to provide frontier molecular orbitals for excited state assignment.

Figure S1. The TPSS-D3/def2-TZVP + COSMO(THF) computed spin densities of various open-shell complexes, plotted at 0.001 density contour. The computed Wiberg indices for changed complexes **4**$^{\bullet+}$ and **4**$^{\bullet-}$ are also compared with those of **4** to reveal bonding changes up redox reaction.

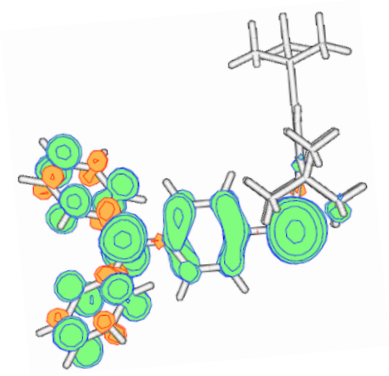




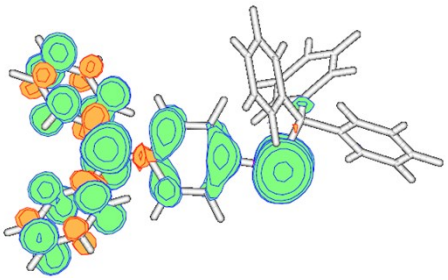
$4^{\bullet+}$



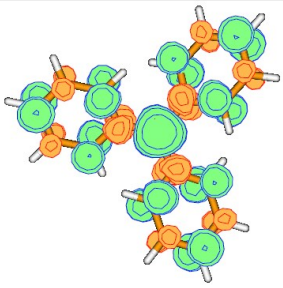
$4^{\bullet-}$



$VIa^{\bullet-}$



$5^{\bullet-}$



$Ph_3C^{\bullet}$

TPSS-D3/def2-TZVP + COSMO(THF)
computed Wiberg bond indices

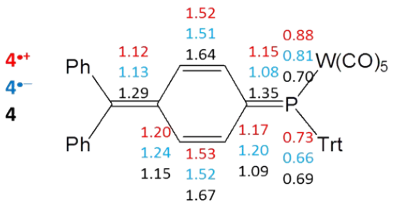


Table S1. TPSS-D3/def2-TZVP + COSMO(THF) computed zero-point energy (ZPE), enthalpic (Hc) and Gibbs free-energy (Gc) corrections; COSMO-RS solvation enthalpic (Hsol) and free-energy (Gsol) corrections in THF (or CH_3CN), shifted by +1.90 kcal/mol to use 1 mol/L reference state concentration; TPSS-D3/def2-TZVP + COSMO(THF) total energy (E_{COS}); TPSS-D3/def2-QZVP single-point energies (E_{TPSS}); the final relative Gibbs free-energies (ΔG) at the TPSS-D3/def2-QZVP + COSMO-RS level. Each structure is labeled either by its molecular formula, or a specific name in bold, followed by the respective superscript of •, +, – and = for radical, singly charged cation, singly and doubly charged anion. Each transition structure (with only one imaginary frequency IF, shown in parentheses) are indicated by the "**TS**" prefix.

Species	IF	ZPE	Hc	Gc	Hsol	Gsol	E_{COS}	E_{TPSS}/QZ	ΔG	ΔG
	cm^{-1}	kcal/mol	kcal/mol	kcal/mol	kcal/mol	kcal/mol	Eh	Eh	kcal/mol	eV
1a$^-$ + $Li(Thf)_4^+$	0	492.69	530.08	422.53	-106.84	-90.14	-3107.48371	-3107.54485	0.0	--
1a$Li(Thf)_3$ + Thf	0	492.67	529.73	426.50	-47.48	-29.12	-3107.50810	-3107.64487	2.2	--
1a$^-$ + Ph_3C^+	0	372.27	402.69	311.12	-109.83	-90.88	-2902.91512	-2902.94943	0.0	--
1a$^\bullet$ + $Ph_3C^\bullet$	0	371.94	402.31	310.95	-42.91	-27.49	-2902.93798	-2903.06047	-6.5	--
2	0	373.91	404.35	328.18	-37.64	-26.78	-2902.97784	-2903.10320	-15.3	--
2c	0	374.39	404.53	329.77	-35.38	-25.37	-2902.96923	-2903.09412	-6.64	
2o	0	373.91	404.28	328.78	-36.31	-25.98	-2902.96624	-2903.09096	-6.26	
TS24	-594	369.42	400.24	322.89	-43.52	-31.47	-2902.90658	-2903.02856	21.5	--
4 + HCl	0	369.79	401.25	313.54	-54.62	-27.52	-2902.93944	-2903.06011	-3.7	--
2 + Et_3N	0	501.18	537.99	434.89	-45.09	-29.47	-3195.56963	-3195.71435	0.0	--
TS24n	-601	502.00	537.64	452.27	-41.93	-30.38	-3195.55621	-3195.70098	24.9	--
2Cl$^-$ + Et_3NH	0	502.61	539.44	436.17	-133.57	-105.68	-3195.54592	-3195.59127	2.3	--
TS4nc	-87	503.19	540.34	451.33	-51.17	-37.40	-3195.58361	-3195.71941	5.3	--
4 + Et_3NHCl	0	502.55	539.60	434.89	-61.64	-43.28	-3195.57948	-3195.70026	-5.0	--
TS34n	-1181	499.62	536.91	447.37	-43.92	-31.83	-3195.57749	-3195.72027	6.4	--
3 + Et_3N	0	501.56	538.46	434.68	-45.69	-29.87	-3195.60050	-3195.74397	-19.2	--
Et_3NH^+ + **s2N**$^-$	0	276.10	293.67	229.39	-117.74	-94.90	-1166.67802	-1166.67792	0.0	--
Et_3N + **s2N**H	0	274.91	292.10	229.46	-16.44	-5.41	-1166.81097	-1166.87298	-32.8	--
Et_3NH^+ + **DBU**	0	289.19	302.34	247.06	-79.42	-58.73	-755.42798	-755.40394	0.0	--
Et_3N + **DBU**H^+	0	288.38	301.59	246.25	-68.21	-50.97	-755.44306	-755.43042	-9.7	--
2 + **s2N**$^-$	0	512.55	554.23	440.65	-88.86	-70.54	-3776.60641	-3776.77805	0.0	--
2Cl$^-$ + **s2NH**$^+$	0	512.78	554.11	442.00	-76.03	-57.26	-3776.71565	-3776.85003	-30.5	--
3 + **s2N**$^-$	0	512.93	554.70	440.44	-89.46	-70.94	-3776.63728	-3776.80766	-19.2	--

2 + $Fc^{\bullet+}$	0	479.45	516.04	413.05	-96.10	-74.08	-4553.96901	-4554.08323	0.0	0.00
2$^{\bullet+}$ + Fc	0	478.88	515.22	414.12	-74.86	-56.27	-4553.95835	-4554.09587	10.9	0.47
3 + $Fc^{\bullet+}$	0	479.83	516.51	412.84	-96.70	-74.48	-4553.99988	-4554.11284	0.0	0.00
3$^{\bullet+}$ + Fc	0	479.04	515.69	413.33	-73.18	-55.47	-4553.95622	-4554.09989	27.6	1.20
$Ph_3C^{\bullet}$ + $Fc^{\bullet+}$	0	277.65	293.58	232.73	-77.17	-59.03	-2384.48218	-2384.50609	0.0	0.00
Ph_3C^{+} + Fc	0	277.85	293.61	234.16	-63.57	-49.05	-2384.49971	-2384.53580	-7.2	-0.31
Ph_3C^{-} + $Fc^{\bullet+}$	0	275.45	291.62	229.91	-115.78	-96.38	-2384.58048	-2384.55727	0.0	0.00
$Ph_3C^{\bullet}$ + Fc	0	276.59	292.36	232.90	-30.20	-17.91	-2384.66709	-2384.74978	-39.3	-1.71
4= + $Fc^{\bullet+}$	0	467.70	503.43	401.97	-204.75	-179.76	-4093.29485	-4093.26023	0.0	0.00
4$^{\bullet-}$ + Fc	0	468.37	503.88	403.70	-78.66	-60.83	-4093.39080	-4093.51457	-38.9	-1.69
4$^{\bullet-}$ + $Fc^{\bullet+}$	0	469.44	505.10	403.54	-125.64	-101.95	-4093.20589	-4093.27088	0.0	0.00
4 + Fc	0	470.12	505.51	405.67	-50.59	-33.95	-4093.27296	-4093.43023	-29.9	-1.29
4 + $Fc^{\bullet+}$	0	471.19	506.73	405.51	-97.56	-75.07	-4093.08805	-4093.18653	0.0	0.00
4$^{\bullet+}$ + Fc	0	470.58	506.01	406.16	-74.70	-56.46	-4093.09295	-4093.21604	0.8	0.03
5= + $Fc^{\bullet+}$	0	441.42	468.55	384.10	-213.96	-189.35	-3458.94561	-3458.86365	0.0	0.00
5$^{\bullet-}$ + Fc	0	442.65	469.36	387.15	-80.78	-63.34	-3459.06777	-3459.15670	-54.8	-2.38
5$^{\bullet-}$ + $Fc^{\bullet+}$	0	443.72	470.58	386.99	-127.76	-104.46	-3458.88286	-3458.91301	0.0	0.00
5 + Fc	0	444.15	470.87	388.49	-48.46	-32.20	-3458.95889	-3459.08701	-35.4	-1.54
5 + $Fc^{\bullet+}$	0	445.22	472.09	388.33	-95.43	-73.33	-3458.77398	-3458.84331	0.0	0.00
5$^{\bullet+}$ + Fc	0	444.97	471.65	389.41	-73.80	-55.83	-3458.77924	-3458.87135	1.0	0.04
VIa= + $Fc^{\bullet+}$	0	532.09	562.89	472.26	-211.90	-187.37	-3429.25541	-3429.18532	0.0	0.00
VIa$^{\bullet-}$ + Fc	0	534.04	564.15	476.52	-76.99	-59.87	-3429.38615	-3429.48640	-57.2	-2.48
VIa$^{\bullet-}$ + $Fc^{\bullet+}$	0	535.11	565.37	476.36	-123.96	-100.99	-3429.20124	-3429.24271	0.0	0.00
VIa + Fc	0	535.39	565.63	477.62	-44.46	-28.67	-3429.28596	-3429.42504	-40.8	-1.77
VIa + $Fc^{\bullet+}$	0	536.46	566.85	477.46	-91.43	-69.79	-3429.10106	-3429.18135	0.0	0.00

VIa$^{\bullet+}$ + Fc	0	536.00	566.06	478.49	-68.80	-52.32	-3429.10851	-3429.21105	-0.1	-0.01

in MeCN	IF	ZPE	Hc	Gc	Hsol	Gsol	E_{COS}	E_{TPSS}	ΔΓ	E
2 + Fc$^{\bullet+}$	0	479.45	516.04	413.05	-80.91	-67.75	-4553.96901	-4554.08323	0.0	0.00
2$^{\bullet+}$ + Fc	0	478.88	515.22	414.12	-60.06	-48.66	-4553.95835	-4554.09587	12.2	0.53
3 + Fc$^{\bullet+}$	0	479.83	516.51	412.84	-81.38	-70.06	-4553.99988	-4554.11284	0.0	0.00
3$^{\bullet+}$ + Fc	0	479.04	515.69	413.33	-59.70	-50.28	-4553.95622	-4554.09989	29.2	1.27
$Ph_3C^{\bullet}$ + Fc$^{\bullet+}$	0	277.65	293.58	231.67	-63.74	-53.58	-2384.48218	-2384.50609	0.0	0.00
Ph_3C^{+} + Fc	0	277.85	293.61	233.09	-51.19	-43.11	-2384.49971	-2384.53580	-6.8	-0.29
Ph_3C^{-} + Fc$^{\bullet+}$	0	275.45	291.62	229.91	-113.05	-96.17	-2384.58048	-2384.55727	0.0	0.00
$Ph_3C^{\bullet}$ + Fc	0	276.59	292.36	231.83	-26.01	-14.73	-2384.66709	-2384.74978	-37.4	-1.62
4 + Fc$^{\bullet+}$	0	471.19	506.73	405.51	-82.20	-70.66	-4093.08805	-4093.18653	0.0	0.00
4$^{\bullet+}$ + Fc	0	470.58	506.01	406.16	-60.25	-50.76	-4093.09295	-4093.21604	2.9	0.12
4$^{\bullet-}$ + Fc$^{\bullet+}$	0	469.44	505.10	403.54	-119.54	-101.11	-4093.20589	-4093.27088	0.0	0.00
4 + Fc	0	470.12	505.51	405.67	-44.48	-31.81	-4093.27296	-4093.43023	-28.4	-1.23

Figure S2. The frontier molecular orbital levels (in eV) of complex **4**, computed at the PBE0/def2-TZVP level and plotted at 0.02 contour.

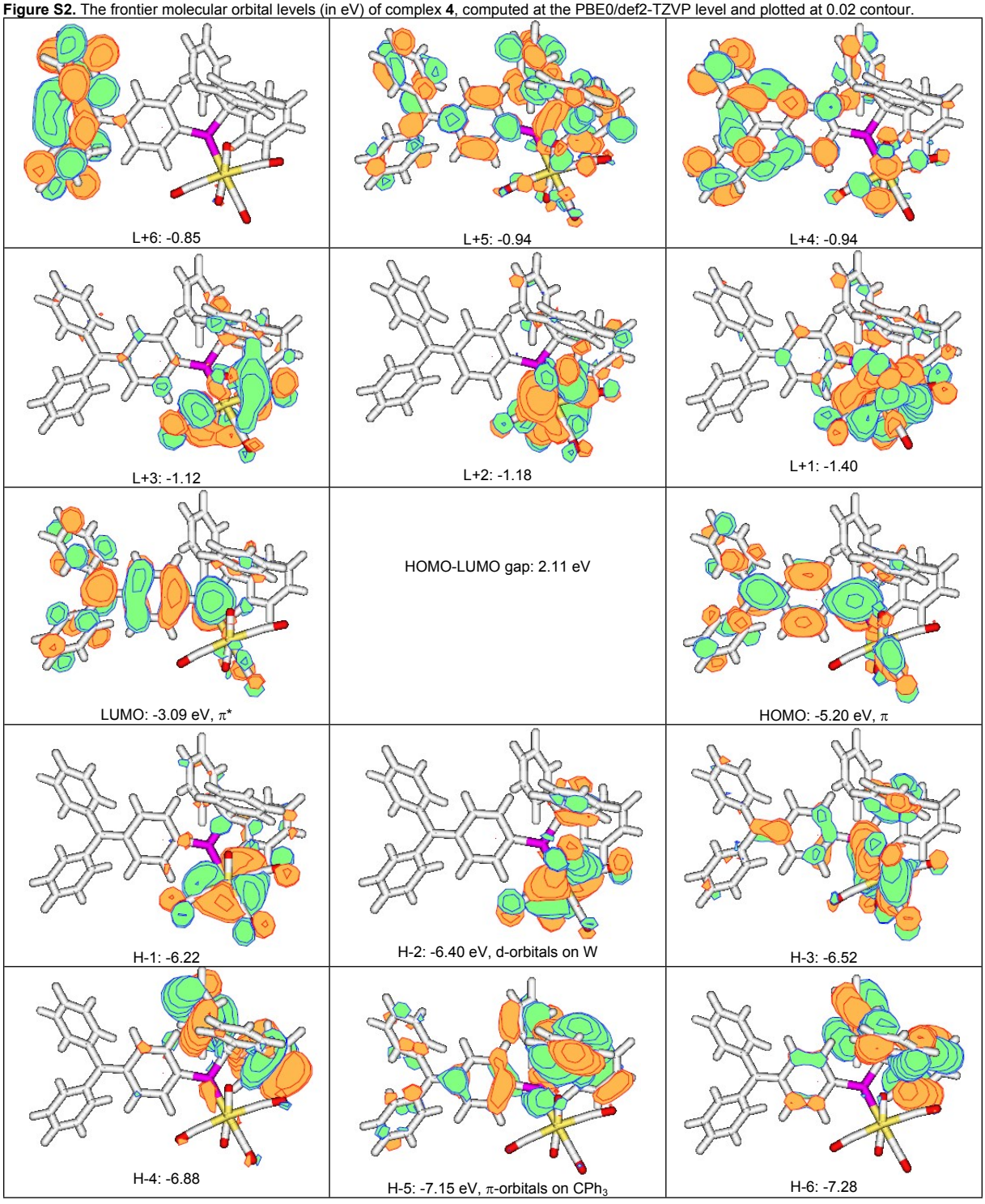


Table S2. TD-DFT PBE0/def2-TZVPD computed 20 lowest excitation energies E (shifted by +0.18 eV), oscillator strengths (Osc), and electronic assignment (leading electronic transition and its ratio) for the ten lowest 13 excited states of phosphaquinone methide complex **4**. For the assignment, H and L stand for the HOMO (occupied orbital 178) and LUMO (unoccupied orbital 179), respectively, while H-1 and L+1 for the second occupied and unoccupied orbitals, and so on.

	TD-DFT						Expt.
States	λ /nm	Osc	E /eV	Assign	Ratio %	Comment	E / eV (rel. Int.)
1	**563.5**	**0.936**	**2.20**	**H → L**	**94.6**	**π → π***	**2.20 (1.0)**
2	494.3	0.044	2.51	H-1 → L	97.1	5d → π* MLCT	
3	455.1	0.002	2.72	H-2 → L	92.2	5d → π* MLCT	
4	**408.7**	**0.166**	**3.03**	**H-3 → L**	**85.3**	**5d → π* MLCT**	**3.69 (1.2)**
5	394.7	0.023	3.14	H → L+1	90.1	π → 6d* LMCT	
6	381.0	0.001	3.25	H → L+2	86.0	π → 6d* LMCT	
7	378.0	0.002	3.28	H-4 → L	96.1	π on CPh_3 → π* CT	
8	365.4	0.009	3.39	H → L+3	86.5	π → 6d* LMCT	
9	349.8	0.042	3.55	H-5 → L	84.0	π on CPh_3 → π* CT	
10	343.9	0.004	3.61	H → L+4	42.8	π → π* on CPh_2 CT	
				H → L+5	40.2	π → π* on CPh_3 CT	
11	352.4	0.002	3.70	H-6- to L	74.9	π on CPh_3 → π* CT	
12	351.0	0.007	3.71	H to L+4	40.8	π → π* on CPh_2 CT	
				H to L+7	22.2		
				H to L+5	18.6	π → π* on CPh_3 CT	
13	345.9	0.004	3.77	H-1 to L+1	29.8	5d → 6d* on W	
				H-2 to L+1	28.6	5d → 6d*	
				H-1 to L+3	15.7	5d → 6d*	
				H-2 to L+3	10.0	5d → 6d*	
14	344.2	0.009	3.78	--	--	--	
15	340.7	0.006	3.82	--	--	--	
16	340.6	0.005	3.82	--	--	--	
17	339.6	0.004	3.83	--	--	--	
18	336.9	0.011	3.86	--	--	--	
19	335.5	0.001	3.88	--	--	--	
20	332.6	0.002	3.91	--	--	--	
							5.21 (7.4)

Table S3. The TPSS-D3/def2-TZVP + COSMO(THF) optimized atomic Cartesian coordinates (in Å). Each structure is labeled either by its molecular formula or a name in bold (see also **Table S1**), followed by the number of atoms, the TPSS-D3/def2-TZVP + COSMO(THF) total energy, and the detailed atomic coordinates (double column list).

1aLi(THF)$_3$.xyz
87
Energy = -2874.915520682

P	-0.2093640	-0.2524859	-0.3687565
Cl	-0.4371624	-0.5258918	-2.4878149
C	-0.3261415	-2.1271113	0.2410054
C	-0.7294442	-2.0182741	1.7106179
C	-0.0875733	-1.0671535	2.5176308
C	-1.6451662	-2.8867120	2.3141434
C	-0.3758419	-0.9576308	3.8752494
H	0.6624909	-0.4189114	2.0692576
C	-1.9235621	-2.7935761	3.6792890
H	-2.1411037	-3.6442618	1.7167072
C	-1.2989651	-1.8244814	4.4640387
H	0.1192017	-0.1978061	4.4734923
H	-2.6369053	-3.4798373	4.1275330
H	-1.5259639	-1.7461326	5.5235153
C	-1.3387435	-2.8964220	-0.5990670
C	-0.9681136	-3.9464247	-1.4476876
C	-2.6952290	-2.5420267	-0.5506692
C	-1.9185347	-4.6122165	-2.2263068
H	0.0705634	-4.2523746	-1.5075178
C	-3.6452183	-3.2006876	-1.3236116
H	-2.9987264	-1.7309843	0.1004890
C	-3.2613882	-4.2437846	-2.1708391
H	-1.6015998	-5.4230043	-2.8771503
H	-4.6867990	-2.8960551	-1.2685319
H	-4.0002046	-4.7600547	-2.7776848
C	1.0693626	-2.7660927	0.1547386
C	1.5272942	-3.6291254	1.1602306
C	1.8947578	-2.5635572	-0.9606648
C	2.7670840	-4.2646490	1.0570993
H	0.9112787	-3.8074924	2.0353526
C	3.1299585	-3.2006304	-1.0705962
H	1.5536865	-1.9124459	-1.7569396
C	3.5759413	-4.0552173	-0.0599339
H	3.0989125	-4.9226216	1.8557409
H	3.7463778	-3.0278588	-1.9488259
H	4.5409938	-4.5475136	-0.1407824
W	-2.1472287	1.3603820	0.2714794
C	-3.3596653	0.6210733	-1.2257154
O	-4.0688902	0.2419084	-2.0571134
C	-3.1710053	0.2299532	1.6540337
O	-3.8190733	-0.3267725	2.4366152
C	-3.4612911	2.8462759	0.6370963
O	-4.2134040	3.7105081	0.8354641
C	-0.9875088	2.0286703	1.8190651
O	-0.3778560	2.4073300	2.7340036
C	-1.2646821	2.5714765	-1.1317674
O	-0.8307273	3.2797221	-1.9419512
Li	2.1740171	0.7931280	-0.2165711
O	3.3803903	0.2757166	-1.6777034
O	2.1102257	2.7595905	-0.4307854
O	3.0338466	0.3745694	1.4999376

C	3.0692262	0.1484147	-3.0924204
C	4.8262497	0.1950382	-1.4925469
C	1.7231801	3.8084227	0.5008685
C	2.5491168	3.3706428	-1.6846689
C	3.7811164	-0.8487339	1.7396017
C	3.0486432	1.1673681	2.7250556
C	4.3319379	0.6045611	-3.8072777
H	2.8372040	-0.9002030	-3.3160895
H	2.1825082	0.7528798	-3.2866351
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H	5.0410951	-0.6534804	-0.8381322
H	5.1453120	1.1203843	-1.0009696
C	2.4357575	5.0578830	0.0055561
H	0.6342271	3.9263129	0.4678803
H	2.0189201	3.4871690	1.4998980
C	2.3465389	4.8762873	-1.5171012
H	1.9541995	2.9460617	-2.4966123
H	3.6025102	3.1092771	-1.8255159
C	3.5239655	-1.1629164	3.2035217
H	3.4052941	-1.5935933	1.0397928
H	4.8471132	-0.6610690	1.5509515
C	3.5585816	0.2381851	3.8423910
H	2.0260914	1.5128998	2.8925045
H	3.7027878	2.0325197	2.5742219
H	4.3911642	0.2252233	-4.8303161
H	4.3801143	1.6981409	-3.8356792
H	5.5891598	-1.0254365	-3.1168656
H	6.3827907	0.5544750	-2.9884380
H	1.9566830	5.9753474	0.3564347
H	3.4801091	5.0579880	0.3363406
H	1.3546936	5.1686972	-1.8742111
H	3.0974782	5.4514448	-2.0641709
H	2.5389095	-1.6239241	3.3149185
H	4.2760218	-1.8349691	3.6243503
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H	4.5828240	0.5044995	4.1186591

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P	1.4298302	-0.6751496	-0.7470396
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C	2.5955462	0.6642479	1.3796331
C	1.2649829	0.8861252	1.7678593
C	3.5902664	0.7716273	2.3604045
C	0.9319850	1.1507956	3.0944870
H	0.4814517	0.8571735	1.0127677
C	3.2638238	1.0578744	3.6863041
H	4.6305290	0.6266650	2.0887869
C	1.9326645	1.2353182	4.0642596
H	-0.1098627	1.2951637	3.3676552
H	4.0557371	1.1344387	4.4269631
H	1.6782714	1.4435010	5.1000102
C	4.2424432	-0.2826552	-0.3481470
C	5.0192053	0.0327309	-1.4735128
C	4.6994275	-1.3134023	0.4870175
C	6.2091068	-0.6432138	-1.7448688
H	4.6849985	0.8136650	-2.1477673
C	5.8902002	-1.9857902	0.2250623
H	4.1127290	-1.5933497	1.3524475
C	6.6566340	-1.6541983	-0.8942720
H	6.7854663	-0.3775187	-2.6277440
H	6.2144708	-2.7788305	0.8939456
H	7.5848079	-2.1800575	-1.1021557
C	2.9047320	1.8058512	-0.7820659
C	3.8202176	2.7685269	-0.3279473
C	2.0401065	2.1582540	-1.8202163
C	3.8693707	4.0411922	-0.8906481
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C	2.0844537	3.4350624	-2.3896891
H	1.3224536	1.4289825	-2.1825261
C	2.9966807	4.3828144	-1.9285397
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H	1.4014385	3.6836260	-3.1982021
H	3.0294900	5.3757868	-2.3692949
W	1.0232909	-2.9116579	0.5313708
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C	1.9945537	-2.4779384	2.2912925
O	2.4933861	-2.3084078	3.3250472
C	0.4960176	-4.6641267	1.3491417
O	0.2003542	-5.6966278	1.8149515
C	-0.6318071	-1.9719720	1.2922157
O	-1.5701223	-1.4321191	1.7130676
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O	-0.6572419	-3.7202506	-2.0862761

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C	2.6962390	0.6565636	1.3947821
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C	3.6690234	0.7700463	2.3940458
C	0.9796801	1.1172609	3.0562010
H	0.5896230	0.8332470	0.9626999
C	3.3001765	1.0466208	3.7106145
H	4.7177221	0.6472172	2.1458541
C	1.9559435	1.2062880	4.0499630
H	-0.0690419	1.2542632	3.3024900
H	4.0686397	1.1321942	4.4734944
H	1.6717089	1.4073286	5.0786619
C	4.4023663	-0.2568665	-0.3163302
C	5.1910062	0.0677111	-1.4294000
C	4.8149449	-1.3193541	0.5054407
C	6.3702487	-0.6270645	-1.6940477
H	4.8785632	0.8657803	-2.0935809
C	5.9920064	-2.0142514	0.2418597
H	4.2099564	-1.6009588	1.3593308
C	6.7782593	-1.6688302	-0.8591429
H	6.9681276	-0.3554981	-2.5593497
H	6.2915653	-2.8290321	0.8944203
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H	2.6521685	5.3630885	-2.3125252
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C	2.4298191	0.4280191	1.4976440
C	1.2058040	-0.0729046	1.9822468
C	3.5705791	0.2268807	2.2879040
C	1.1276283	-0.7154144	3.2162418
H	0.3079896	0.0217132	1.3865899
C	3.4938137	-0.4236863	3.5201488
H	4.5339348	0.5781515	1.9396477
C	2.2704986	-0.8934800	3.9952909
H	0.1672114	-1.0912372	3.5575274
H	4.3990540	-0.5652356	4.1041887
H	2.2103155	-1.4024975	4.9531837
C	3.9520536	1.6196238	-0.1349795
C	4.3543251	2.7618400	0.5786991
C	4.8709882	1.0346763	-1.0046772
C	5.6344100	3.2876683	0.4355922
H	3.6495685	3.2381482	1.2545032
C	6.1569575	1.5603480	-1.1580843
H	4.5907695	0.1618983	-1.5788387
C	6.5463053	2.6868413	-0.4383536
H	5.9206327	4.1688720	1.0035391
H	6.8494937	1.0827577	-1.8458292
H	7.5455625	3.0968793	-0.5562192
C	1.5712603	2.2823882	-0.0889450
C	0.5493871	2.6310797	0.8012615
C	1.7470672	3.0871257	-1.2288658
C	-0.3073254	3.7000242	0.5324730
H	0.4102534	2.0754010	1.7191700
C	0.8883212	4.1467539	-1.5049231
H	2.5650732	2.8739850	-1.9060397
C	-0.1575238	4.4518690	-0.6303021
H	-1.0990641	3.9359200	1.2381134
H	1.0394738	4.7377794	-2.4043536
H	-0.8335311	5.2746348	-0.8457885
W	3.3683129	-2.6078631	-0.8771891
C	4.4141240	-2.1260931	-2.5799447
O	5.0397297	-1.9042278	-3.5287018
C	4.9459865	-1.9185884	0.2517467
O	5.8910511	-1.6315979	0.8553129
C	4.2766477	-4.3981415	-0.8881294
O	4.7901677	-5.4440268	-0.9001095
C	2.4252342	-3.1815591	0.8674530
O	1.9557196	-3.5821963	1.8443602
C	1.8860356	-3.3952841	-2.0764567
O	1.1024777	-3.8741483	-2.7781872
C	0.2671806	-0.5491823	-0.9815903
C	-0.3420306	-1.7170082	-0.4478279
C	-0.6150033	0.4975289	-1.3763066
C	-1.6979607	-1.8060530	-0.2535355
H	0.2826130	-2.5571032	-0.1638994
C	-1.9739180	0.3953956	-1.2123958
H	-0.2077199	1.4034536	-1.8111549
C	-2.6021601	-0.7463286	-0.6074991
H	-2.1038051	-2.7250780	0.1577106
H	-2.5928730	1.2358903	-1.5087250
C	-3.9997963	-0.8220195	-0.3812610
C	-4.5593683	-1.7495073	0.6051527
C	-5.8138845	-2.3749299	0.4044246
C	-3.8989176	-2.0457421	1.8222828
C	-6.3627321	-3.2416048	1.3451977
H	-6.3561902	-2.1720357	-0.5152200
C	-4.4443482	-2.9156373	2.7615266
H	-2.9489019	-1.5615374	2.0305237
C	-5.6829122	-3.5273158	2.5346581
H	-7.3253062	-3.7078136	1.1450806
H	-3.9065246	-3.1079104	3.6876828
H	-6.1095274	-4.2054803	3.2687847
C	-4.9345294	0.0353319	-1.1174488
C	-4.7465976	0.3548641	-2.4827706
C	-6.0905271	0.5685399	-0.4999412
C	-5.6400463	1.1657005	-3.1766749
H	-3.8860843	-0.0587828	-3.0015579
C	-6.9887129	1.3735474	-1.1939686
H	-6.2717384	0.3449935	0.5480937
C	-6.7723232	1.6862200	-2.5406825
H	-5.4605261	1.3810702	-4.2279905
H	-7.8603495	1.7710875	-0.6778723
H	-7.4721812	2.3166039	-3.0828963

2c.xyz
81
Energy = -2902.969227631

P	-0.1563915	-0.0001919	-0.4584887
Cl	-0.2464224	-0.0636322	-2.5549422
C	-1.5727210	1.3396713	0.0466070
C	-1.6311202	1.0791155	1.5541843
C	-2.5437476	0.1617173	2.0985699
C	-0.7329552	1.7076557	2.4308488
C	-2.5655726	-0.1091479	3.4640565
H	-3.2494055	-0.3408184	1.4521001
C	-0.7543605	1.4405603	3.7992379
H	-0.0227351	2.4259114	2.0411036
C	-1.6716053	0.5302369	4.3230620
H	-3.2807513	-0.8283132	3.8515705
H	-0.0468590	1.9412188	4.4521556
H	-1.6872188	0.3199226	5.3883924
C	-1.0571588	2.7588833	-0.2911755
C	-1.5245471	3.8238510	0.4954306
C	-0.3236734	3.0684587	-1.4423896
C	-1.2440756	5.1449843	0.1582573
H	-2.1303334	3.6193282	1.3718225
C	-0.0478497	4.3921657	-1.7862569
H	0.0380717	2.2820756	-2.0899421
C	-0.5004685	5.4382469	-0.9867219
H	-1.6169912	5.9467875	0.7893881
H	0.5313649	4.5976211	-2.6819583
H	-0.2818789	6.4687646	-1.2509586
C	-2.9649909	1.3443165	-0.6286622
C	-4.1181113	1.5949524	0.1308073
C	-3.1060242	1.3434698	-2.0239745
C	-5.3683846	1.7330775	-0.4708504
H	-4.0525587	1.7019992	1.2059353
C	-4.3548187	1.4632724	-2.6284524
H	-2.2335281	1.2565716	-2.6540921
C	-5.5020296	1.6422849	-1.8546383
H	-6.2381812	1.9171506	0.1536172
H	-4.4245511	1.4331997	-3.7123315
H	-6.4768993	1.7374480	-2.3240734
W	2.3143720	0.7203168	0.2357319
C	1.9890274	2.7494448	0.4141871

O	2.0023340	3.8813412	0.6507524
C	2.2237166	0.6934632	2.2911984
O	2.3372977	0.7329057	3.4410893
C	4.2349545	1.2358977	0.4746382
O	5.3500786	1.5332763	0.5909175
C	3.0435146	-1.1954192	0.4068811
O	3.6089247	-2.1883044	0.5881429
C	2.6843842	0.8454884	-1.7883438
O	2.9867314	0.9492813	-2.8987209
C	-4.8906533	-2.4772174	0.4734213
C	-4.4089212	-1.8204379	-0.6607911
C	-3.9866117	-2.9978999	1.3999889
H	-5.9598260	-2.5903541	0.6280550
C	-3.0378934	-1.6706086	-0.8479923
H	-5.0964376	-1.4152842	-1.3963829
C	-2.6129915	-2.8345376	1.2150142
H	-4.3483326	-3.5261211	2.2774529
C	-2.1220455	-2.1441526	0.0999326
H	-2.6706147	-1.1817076	-1.7425574
H	-1.9253736	-3.2295419	1.9536478
C	-0.6273880	-1.9750735	-0.1460663
C	-0.1973454	-2.7552746	-1.3983580
C	-1.0616228	-3.6351218	-2.0583308
C	1.1292378	-2.6810478	-1.8482233
C	-0.6160856	-4.4010971	-3.1399288
H	-2.0865076	-3.7462175	-1.7261558
C	1.5762430	-3.4327459	-2.9269392
H	1.8142215	-2.0028606	-1.3544597
C	0.7004082	-4.3023361	-3.5830816
H	-1.3080356	-5.0805525	-3.6296060
H	2.6075618	-3.3411923	-3.2554501
H	1.0440778	-4.8967649	-4.4247906
C	0.1821333	-2.4651028	1.0571119
C	0.7286405	-3.7572452	1.0553533
C	0.2748943	-1.7149693	2.2345350
C	1.3603742	-4.2704751	2.1874148
H	0.6536114	-4.3745946	0.1680535
C	0.9041955	-2.2250822	3.3685747
H	-0.1597201	-0.7241439	2.2777184
C	1.4558171	-3.5053821	3.3495898
H	1.7774285	-5.2730280	2.1566444
H	0.9631793	-1.6142302	4.2637070
H	1.9512814	-3.9030234	4.2306835

2o.xyz
81
Energy = -2902.966242338

P	0.7351471	0.2231375	-0.9651077
Cl	1.6518012	0.3369817	-2.8129508
C	2.1218215	1.0295487	0.1921564
C	1.7452691	0.6396676	1.6333763
C	0.4103202	0.5448608	2.0503856
C	2.7446866	0.3963526	2.5854102
C	0.0821253	0.2054960	3.3621716
H	-0.4047915	0.7393260	1.3607562
C	2.4212515	0.0680409	3.9009226
H	3.7878600	0.4526136	2.2976509
C	1.0875819	-0.0362360	4.2956104
H	-0.9622762	0.1343805	3.6448054
H	3.2187056	-0.1171652	4.6148735
H	0.8352607	-0.3041357	5.3174497
C	3.5176067	0.4666300	-0.1311118
C	4.6600250	1.2477986	0.1047881
C	3.7091196	-0.8563937	-0.5317931
C	5.9397444	0.7239871	-0.0785287
H	4.5547298	2.2710514	0.4475405
C	4.9831450	-1.3852654	-0.7269208
H	2.8455266	-1.4875665	-0.6935634
C	6.1096787	-0.5940435	-0.5039018
H	6.8047191	1.3518706	0.1160442
H	5.0906936	-2.4160823	-1.0522634
H	7.1060660	-0.9995876	-0.6539391
C	2.0984055	2.5459785	-0.0195887
C	1.4375691	3.4061366	0.8658650
C	2.7468366	3.1085999	-1.1330672
C	1.4079265	4.7832321	0.6382853
H	0.9425426	3.0032748	1.7433595
C	2.7348848	4.4841121	-1.3499791
H	3.2658543	2.4630947	-1.8318094
C	2.0581967	5.3296570	-0.4677191
H	0.8842862	5.4286219	1.3374227
H	3.2467135	4.8940059	-2.2158785
H	2.0425519	6.4020651	-0.6387020
W	-0.0344566	-2.2097823	-0.5679388
C	1.4109463	-2.9183545	-1.8493307
O	2.1867887	-3.3854456	-2.5680135
C	1.2243049	-2.5075810	1.0426364
O	1.9109290	-2.7815031	1.9288295
C	-0.6341921	-4.1214253	-0.3397573
O	-0.9842219	-5.2186086	-0.2120024
C	-1.5070432	-1.7499695	0.7994062
O	-2.3058525	-1.6513041	1.6292796
C	-1.2332411	-2.1471245	-2.2383044
O	-1.8651525	-2.2474484	-3.2019726
C	-0.7721043	2.4765238	-3.3714546
C	-1.7296517	1.4225380	-3.6206578
C	-0.2571888	2.6537405	-2.1367344
H	-0.4977995	3.1434860	-4.1841060
C	-2.3414803	0.7858460	-2.5854393
H	-2.0534484	1.2285589	-4.6390339
C	-0.5979761	1.6837003	-1.0580179
H	0.4398325	3.4504295	-1.9150110
C	-1.9920487	1.1307739	-1.2184695
H	-3.1878234	0.1400684	-2.7802183
H	-0.4513191	2.1295005	-0.0761623
C	-2.9155858	1.1339183	-0.1968167
C	-4.2259870	0.4493228	-0.3247352
C	-5.4040236	1.1141577	0.0590874
C	-4.3329827	-0.8648278	-0.8062357
C	-6.6457194	0.4938391	-0.0603914
H	-5.3409774	2.1282610	0.4427330
C	-5.5713970	-1.4913361	-0.9154717
H	-3.4298166	-1.4035105	-1.0707171
C	-6.7353140	-0.8122580	-0.5477337
H	-7.5449326	1.0300707	0.2297691
H	-5.6279216	-2.5134821	-1.2792233
H	-7.7023287	-1.2997098	-0.6320070
C	-2.7330907	1.9225175	1.0460728
C	-2.2271842	3.2363399	1.0146687
C	-3.1524930	1.4047991	2.2847621
C	-2.0897630	3.9775632	2.1853658
H	-1.9716544	3.6865052	0.0599472
C	-3.0127408	2.1463105	3.4550442
H	-3.5784863	0.4085290	2.3240339
C	-2.4692805	3.4315614	3.4132673
H	-1.7030891	4.9913877	2.1359878
H	-3.3290143	1.7191627	4.4025397
H	-2.3627459	4.0111237	4.3255827

2.xyz
81
Energy = -2902.977843096

P	1.5498666	-0.7190211	-0.8618873
Cl	2.4233204	-1.4419820	-2.6182399
C	2.9764960	0.4646576	-0.1646025
C	2.7394672	0.5761996	1.3450003
C	1.4467604	0.7251062	1.8632998
C	3.8191227	0.6326541	2.2347986
C	1.2292014	0.9066957	3.2273684
H	0.5904645	0.7144947	1.1953689
C	3.6072104	0.8208896	3.6009791
H	4.8320281	0.5353569	1.8598256
C	2.3126377	0.9527934	4.1045459
H	0.2141038	1.0063782	3.6004274
H	4.4599894	0.8617223	4.2725401
H	2.1498973	1.0890809	5.1696436
C	4.3093066	-0.2401938	-0.4446506
C	5.3460930	0.3514400	-1.1722877
C	4.5238637	-1.5171403	0.0935397
C	6.5490977	-0.3288633	-1.3804556
H	5.2314944	1.3520677	-1.5717085
C	5.7139501	-2.2030482	-0.1205712
H	3.7443608	-1.9707903	0.6950197
C	6.7358135	-1.6107339	-0.8668224
H	7.3415164	0.1534208	-1.9459466
H	5.8453208	-3.1963768	0.2984184
H	7.6692877	-2.1397614	-1.0356441
C	2.8811602	1.8379164	-0.8371938
C	2.7109166	3.0078085	-0.0850768
C	2.9861141	1.9621087	-2.2332796
C	2.6229336	4.2552102	-0.7067702
H	2.6433710	2.9506003	0.9954590
C	2.8932502	3.2048742	-2.8553667
H	3.1493093	1.0765294	-2.8386008
C	2.7057010	4.3601941	-2.0939135
H	2.4882469	5.1447869	-0.0983920
H	2.9712168	3.2683546	-3.9368732
H	2.6324716	5.3299505	-2.5773344
W	0.6510259	-2.7059607	0.4628754
C	2.1818027	-3.8868488	-0.2461727
O	3.0208622	-4.5881440	-0.6177935
C	1.7525469	-2.4036955	2.1809805
O	2.3506793	-2.3593393	3.1683124
C	-0.1403083	-4.3307434	1.3675420
O	-0.6065390	-5.2640631	1.8706655
C	-0.8647799	-1.6000829	1.3245164
O	-1.6956513	-1.0517312	1.9108151
C	-0.4230902	-3.2873901	-1.1981943
O	-0.9922139	-3.7540624	-2.0904191
C	0.2497854	0.4111852	-1.7426158
C	-0.7491331	-0.4756237	-2.3994369
C	-0.3767792	1.3956033	-0.8170029
H	0.8811502	0.9163608	-2.4832681
C	-2.0310112	-0.5482081	-1.9871043
H	-0.4095551	-1.0772184	-3.2364502
C	-1.6730696	1.3318892	-0.4528251
H	0.2565132	2.1892483	-0.4352299
C	-2.5722043	0.2945662	-0.9334529
H	-2.7118631	-1.2185745	-2.5021511
H	-2.0579866	2.0616071	0.2513911
C	-3.8469695	0.1260365	-0.4308446
C	-4.6286885	-1.0989800	-0.6887419
C	-6.0113186	-1.0251191	-0.9422425
C	-4.0295341	-2.3708586	-0.6410104
C	-6.7566101	-2.1777836	-1.1759290
H	-6.4939706	-0.0522890	-0.9667030
C	-4.7757867	-3.5247910	-0.8657811
H	-2.9752296	-2.4472388	-0.3965646
C	-6.1420394	-3.4329885	-1.1409206
H	-7.8198512	-2.0986045	-1.3849951
H	-4.2930621	-4.4968615	-0.8160261
H	-6.7258578	-4.3321782	-1.3156238
C	-4.4920872	1.1395634	0.4318891
C	-4.5188521	2.4984477	0.0729368
C	-5.1299317	0.7509747	1.6230029
C	-5.1428321	3.4402990	0.8891943
H	-4.0659910	2.8071430	-0.8651632
C	-5.7439994	1.6928115	2.4443375
H	-5.1249489	-0.2978797	1.9053004
C	-5.7518032	3.0422502	2.0812585
H	-5.1614666	4.4845797	0.5896832
H	-6.2176779	1.3749820	3.3690741
H	-6.2370351	3.7763305	2.7182703

2•+.xyz
81
Energy = -2902.782276695

P	1.5657289	-0.7463922	-0.8121853
Cl	2.3434130	-1.3652417	-2.6336860
C	2.9990615	0.4605957	-0.1302473
C	2.8049500	0.5056916	1.3863133
C	1.5285449	0.6254744	1.9512934
C	3.9128534	0.5301396	2.2429931
C	1.3512326	0.7495901	3.3270544
H	0.6517092	0.6323753	1.3116222
C	3.7418038	0.6634615	3.6208724
H	4.9138941	0.4555813	1.8333314
C	2.4628110	0.7678117	4.1692629
H	0.3490272	0.8287252	3.7371432
H	4.6144926	0.6841294	4.2665851
H	2.3334488	0.8628491	5.2429995
C	4.3069826	-0.2467515	-0.4896690
C	5.3056159	0.3468909	-1.2688240
C	4.5375846	-1.5343529	0.0198292
C	6.4860613	-0.3425012	-1.5534839
H	5.1826759	1.3564930	-1.6414428
C	5.7052012	-2.2291398	-0.2731717
H	3.7939388	-1.9861979	0.6664414
C	6.6862586	-1.6351838	-1.0704518
H	7.2524637	0.1406620	-2.1522208
H	5.8528660	-3.2279194	0.1259856
H	7.6028998	-2.1700784	-1.2998529
C	2.8581446	1.8447662	-0.7586629
C	2.6730297	2.9842327	0.0362619
C	2.9237622	2.0157076	-2.1544124
C	2.5303037	4.2465508	-0.5426683
H	2.6420795	2.8906628	1.1158390
C	2.7742520	3.2747226	-2.7325211
H	3.1047418	1.1583012	-2.7942505
C	2.5702974	4.3970989	-1.9282771
H	2.3898603	5.1126096	0.0971894
H	2.8239567	3.3755856	-3.8124004
H	2.4554059	5.3789859	-2.3770281
W	0.6682460	-2.7360175	0.4456986
C	2.1884758	-3.8993250	-0.3417365
O	3.0180293	-4.5780937	-0.7610059
C	1.8130301	-2.4930079	2.1563987
O	2.4349328	-2.4779663	3.1254764
C	-0.1085589	-4.3991863	1.3154291
O	-0.5669407	-5.3459983	1.7922119
C	-0.8113867	-1.6442586	1.3741544
O	-1.6220629	-1.0800892	1.9748979
C	-0.4208767	-3.2453195	-1.2242173
O	-1.0017707	-3.6411894	-2.1415866

C	0.2065118	0.4896339	-1.6351400
C	-0.7489900	-0.3640857	-2.3417142
C	-0.3824181	1.3894464	-0.6412105
H	0.9076531	1.0099199	-2.3015317
C	-2.0472955	-0.4679580	-1.9394602
H	-0.3957382	-0.9310995	-3.1957357
C	-1.6869784	1.2886717	-0.2677653
H	0.2576373	2.1456649	-0.2003471
C	-2.5622877	0.3165660	-0.8580312
H	-2.7266519	-1.1122187	-2.4861810
H	-2.0737616	1.9319239	0.5145163
C	-3.9003590	0.1489739	-0.3919333
C	-4.5904137	-1.1170682	-0.5698053
C	-5.9904120	-1.1460062	-0.7755881
C	-3.8900380	-2.3448383	-0.5192287
C	-6.6516875	-2.3541991	-0.9473075
H	-6.5365018	-0.2109705	-0.8426541
C	-4.5590505	-3.5495278	-0.6699605
H	-2.8257931	-2.3389227	-0.3125568
C	-5.9411240	-3.5581366	-0.8912714
H	-7.7210627	-2.3624742	-1.1320571
H	-4.0123318	-4.4851476	-0.6077727
H	-6.4627791	-4.5017597	-1.0173670
C	-4.5935905	1.2324885	0.2889810
C	-4.4408328	2.5738812	-0.1311486
C	-5.4517339	0.9540732	1.3776665
C	-5.1221265	3.5955190	0.5153450
H	-3.8251426	2.7939691	-0.9978368
C	-6.1100966	1.9842115	2.0361096
H	-5.5570564	-0.0695341	1.7219365
C	-5.9509633	3.3051092	1.6054851
H	-5.0186905	4.6186460	0.1681546
H	-6.7442041	1.7618274	2.8883464
H	-6.4741617	4.1079368	2.1157819

3.xyz
81
Energy = -2903.008708523

P	2.1899673	-1.0170988	-0.6227500
Cl	2.3798997	-1.4808514	-2.6575852
C	2.1933399	0.9359841	-0.5279566
C	2.0217001	1.1344127	0.9895599
C	0.8103332	0.8471580	1.6453745
C	3.0996482	1.5649106	1.7789526
C	0.6729085	1.0206863	3.0209425
H	-0.0398786	0.4856620	1.0852054
C	2.9658575	1.7322315	3.1563821
H	4.0510144	1.7861450	1.3121657
C	1.7491892	1.4688206	3.7849269
H	-0.2808995	0.7970875	3.4898995
H	3.8197000	2.0695419	3.7366894
H	1.6448314	1.6008334	4.8577338
C	3.5235555	1.5266666	-1.0203333
C	3.6412427	2.9263651	-0.9822223
C	4.5952722	0.7875944	-1.5186485
C	4.8032546	3.5595352	-1.4091213
H	2.8095092	3.5187087	-0.6112418
C	5.7641577	1.4191779	-1.9541897
H	4.5363508	-0.2918800	-1.5795524
C	5.8750350	2.8052855	-1.8982270
H	4.8723086	4.6427559	-1.3646091
H	6.5835747	0.8181766	-2.3378079
H	6.7825839	3.2974871	-2.2355416
C	1.0860421	1.5510863	-1.3972855
C	-0.0515572	2.1898674	-0.8884856
C	1.2525859	1.5277959	-2.7932676
C	-1.0269482	2.7098606	-1.7414407
H	-0.1811977	2.3103535	0.1787700
C	0.2755931	2.0331455	-3.6457612
H	2.1616728	1.1155685	-3.2138412
C	-0.8833269	2.6121859	-3.1234117
H	-1.8997383	3.1970282	-1.3154574
H	0.4260641	1.9839766	-4.7204434
H	-1.6479631	3.0065192	-3.7862591
W	3.8647334	-2.3736782	0.7499125
C	4.9407312	-2.7881195	-0.9564755
O	5.5792779	-3.0286807	-1.8885700
C	5.1972651	-0.8538437	1.1668615
O	6.0123555	-0.0804545	1.4337001
C	5.0808396	-3.6125662	1.7781477
O	5.7654258	-4.3400293	2.3683331
C	2.9155572	-1.9647690	2.5359419
O	2.4470872	-1.7822431	3.5752465
C	2.6499356	-3.9897524	0.3534130
O	2.0069507	-4.9244250	0.1346873
C	0.4330914	-1.4385759	-0.4127754
C	0.0126723	-2.0700335	0.7669803
C	-0.5338266	-1.0416695	-1.3483855
C	-1.3405760	-2.2101804	1.0477757
H	0.7457653	-2.4123395	1.4871553
C	-1.8872213	-1.1909152	-1.0629617
H	-0.2341189	-0.5971496	-2.2899334
C	-2.3078758	-1.7305932	0.1567432
H	-1.6496978	-2.6630291	1.9860621
H	-2.6251534	-0.8544890	-1.7847741
C	-4.0061341	-0.5180732	1.5181325
C	-4.9244866	-0.6384860	2.5672113
C	-3.3396290	0.7007645	1.3448154
C	-5.1716605	0.4335322	3.4254403
H	-5.4465752	-1.5813017	2.7137900
C	-3.5850219	1.7754735	2.2000125
H	-2.6194124	0.8090372	0.5387562
C	-4.5012500	1.6454552	3.2448816
H	-5.8834575	0.3203894	4.2385965
H	-3.0559037	2.7133696	2.0533009
H	-4.6877827	2.4789500	3.9160714
C	-4.7249373	-1.7409145	-0.6009444
C	-4.9231361	-2.9563665	-1.2697871
C	-5.3800191	-0.5996311	-1.0718893
C	-5.7534673	-3.0292395	-2.3867274
H	-4.4184542	-3.8509398	-0.9115598
C	-6.2101373	-0.6680616	-2.1937519
H	-5.2437759	0.3475886	-0.5585099
C	-6.3992785	-1.8814919	-2.8548719
H	-5.8983265	-3.9807342	-2.8911187
H	-6.7113190	0.2289114	-2.5472879
H	-7.0473640	-1.9356816	-3.7251028
C	-3.7680145	-1.7051992	0.5864375
H	-3.9493575	-2.6125985	1.1758582

3•+.xyz
81
Energy = -2902.780141446

P	2.1367406	-1.0197744	-0.7161071
Cl	2.3230166	-1.5348120	-2.7172367
C	2.1521169	0.9681338	-0.5894588
C	1.9056128	1.1417575	0.9132960
C	0.6524622	0.8702347	1.4939361
C	2.9410504	1.5665593	1.7637400
C	0.4345078	1.0517853	2.8574285
H	-0.1664837	0.5179162	0.8827599
C	2.7231856	1.7478398	3.1273233
H	3.9174995	1.7926319	1.3546725
C	1.4674693	1.4955461	3.6815096
H	-0.5472230	0.8392255	3.2694693
H	3.5385614	2.0925074	3.7554789
H	1.2993382	1.6377802	4.7443376
C	3.5249366	1.4888166	-1.0150245
C	3.7248726	2.8780934	-0.9283767
C	4.5777033	0.6944365	-1.4857059
C	4.9601477	3.4343200	-1.2323680
H	2.9112959	3.5126609	-0.5897687
C	5.8221977	1.2503676	-1.7945506
H	4.4220442	-0.3604805	-1.6809975
C	6.0193121	2.6198745	-1.6609386
H	5.1053495	4.5053439	-1.1308052
H	6.6196323	0.6116594	-2.1605847
H	6.9799585	3.0610164	-1.9069737
C	1.1121189	1.5760416	-1.5111272
C	-0.0364509	2.2531671	-1.0627569
C	1.3493188	1.5203410	-2.9020721
H	-0.9459636	2.7863397	-1.9701298
H	-0.2038443	2.4039349	-0.0045542
C	0.4354029	2.0427116	-3.8072262
H	2.2618674	1.0664110	-3.2692749
C	-0.7298849	2.6628680	-3.3455831
H	-1.8194691	3.3157496	-1.6019466
H	0.6333990	1.9746724	-4.8720823
H	-1.4472166	3.0712502	-4.0505760
W	3.9567924	-2.1852842	0.6299115
C	5.1128470	-2.6635109	-1.0254244
O	5.7678156	-2.9494873	-1.9237213
C	5.2892764	-0.6837150	1.2266921
O	6.0669537	0.0670709	1.6075400
C	5.0083211	-3.5284600	1.7681994
O	5.5568168	-4.3080384	2.4085464
C	2.9184538	-1.7480643	2.3680064
O	2.4068595	-1.5627405	3.3791948
C	2.7962706	-3.8268713	0.0962581
O	2.1933072	-4.7535001	-0.2074065
C	0.4114124	-1.4697465	-0.4436291
C	0.0231174	-2.1211651	0.7367881
C	-0.5730063	-1.0424186	-1.3486859
C	-1.3238516	-2.2533124	1.0459567
H	0.7669037	-2.4941157	1.4301905
C	-1.9184011	-1.1848100	-1.0299142
H	-0.2921270	-0.5862317	-2.2914431
C	-2.3100590	-1.7461771	0.1907680
H	-1.6133535	-2.7235136	1.9819119
H	-2.6734696	-0.8349455	-1.7267878
C	-3.9775991	-0.5691173	1.6168124
C	-4.8362018	-0.7298902	2.7092261
C	-3.3520694	0.6691736	1.4297613
C	-5.0644202	0.3208835	3.5968125
H	-5.3294611	-1.6867511	2.8636765
C	-3.5802811	1.7232932	2.3139739
H	-2.6810355	0.8115312	0.5872053
C	-4.4357468	1.5515632	3.4023655
H	-5.7306719	0.1771330	4.4426227
H	-3.0851421	2.6770629	2.1539137
H	-4.6093499	2.3692355	4.0956388
C	-4.7444466	-1.7460033	-0.5143397
C	-4.9694444	-2.9518091	-1.1907774
C	-5.3986657	-0.5932488	-0.9565662
C	-5.8248295	-3.0044031	-2.2887300
H	-4.4650529	-3.8550519	-0.8542433
C	-6.2542123	-0.6427876	-2.0590201
H	-5.2466339	0.3455333	-0.4325638
C	-6.4689564	-1.8462325	-2.7287514
H	-5.9909913	-3.9485407	-2.7996738
H	-6.7566546	0.2617906	-2.3898319
H	-7.1376686	-1.8847115	-3.5836695
C	-3.7605878	-1.7325466	0.6512591
H	-3.9253393	-2.6539954	1.2242220

4=.xyz
79
Energy = -2442.303678284

P	2.0109383	-0.7106025	-1.3167892
C	2.5281117	0.9028829	-0.2891480
C	2.1709688	0.6608935	1.1641570
C	0.8330938	0.7357661	1.5985463
C	3.1311966	0.2686571	2.1123980
C	0.4831268	0.4512899	2.9174757
H	0.0562215	1.0101467	0.8946883
C	2.7834393	-0.0120875	3.4322197
H	4.1686308	0.1819470	1.8143520
C	1.4541225	0.0804881	3.8480614
H	-0.5609519	0.5138603	3.2131961
H	3.5563284	-0.3168615	4.1340464
H	1.1792709	-0.1443582	4.8754642
C	4.0192737	1.1913687	-0.5162734
C	4.6772226	2.1268868	0.2975354
C	4.7333930	0.6397894	-1.5850062
C	6.0111288	2.4639155	0.0784217
H	4.1324168	2.5949717	1.1125987
C	6.0697051	0.9737881	-1.8117211
H	4.2296497	-0.0572266	-2.2480655
C	6.7197988	1.8809906	-0.9760989
H	6.4980153	3.1859220	0.7298336
H	6.6021079	0.5168259	-2.6424183
H	7.7621646	2.1385132	-1.1464290
C	1.8153885	2.1186820	-0.9117844
C	1.2364726	3.1353046	-0.1431158
C	1.8425725	2.2894177	-2.3049784
C	0.6521910	4.2527483	-0.7458268
H	1.2347694	3.0563039	0.9384542
C	1.2658101	3.4021606	-2.9109314
H	2.3074011	1.5154802	-2.9085523
C	0.6521595	4.3885010	-2.1331713
H	0.1947861	5.0176109	-0.1225113
H	1.2912239	3.4983328	-3.9939637
H	0.1894839	5.2528527	-2.6029029
W	3.3167785	-2.8586695	-0.4719201
C	4.2476431	-2.7714726	-2.2931750
O	4.7988868	-2.7306932	-3.3170483
C	4.9394591	-1.9057801	0.3462343
O	5.9019674	-1.4581588	0.8215824
C	4.1982024	-4.6037503	-0.0813501
O	4.6991132	-5.6407341	0.1530921
C	2.4597096	-2.9402881	1.4029059
O	2.0425638	-3.0801713	2.4759608
C	1.7154597	-3.8277608	-1.3258832
O	0.8431344	-4.4050017	-1.8291987
C	0.2303210	-0.8071077	-0.9138456
C	-0.3454887	-1.6834371	0.0246080
C	-0.6687908	0.0648275	-1.5707157
C	-1.7040986	-1.6812507	0.3040914
H	0.2950516	-2.3808198	0.5527702
C	-2.0232175	0.0894684	-1.2744982
H	-0.2803166	0.7673372	-2.3033651
C	-2.6078621	-0.7787364	-0.3136948
H	-2.0898431	-2.3867832	1.0363576
H	-2.6583662	0.8128539	-1.7794740

C	-4.0260944	-0.7355926	0.0216716
C	-4.4442761	-1.0066714	1.3828960
C	-5.7338500	-1.5176688	1.7137224
C	-3.5836253	-0.7815434	2.4977555
C	-6.1221907	-1.7713600	3.0244774
H	-6.4305849	-1.7347369	0.9086122
C	-3.9728871	-1.0390461	3.8058601
H	-2.5901393	-0.3859642	2.3103288
C	-5.2515859	-1.5372371	4.0986769
H	-7.1168358	-2.1738904	3.2123257
H	-3.2722425	-0.8373739	4.6151875
H	-5.5560371	-1.7375208	5.1225982
C	-4.9935410	-0.3879559	-0.9999837
C	-4.7611922	-0.6500859	-2.3822005
C	-6.2358136	0.2480179	-0.7099074
C	-5.6758727	-0.3099280	-3.3709519
H	-3.8354344	-1.1432515	-2.6660104
C	-7.1514064	0.5835058	-1.7003631
H	-6.4637526	0.4985100	0.3224725
C	-6.8920165	0.3117342	-3.0514620
H	-5.4448932	-0.5456342	-4.4089991
H	-8.0785984	1.0803199	-1.4169330
H	-7.6090688	0.5743409	-3.8249676

4$^{\bullet-}$.xyz
79
Energy = -2442.214720294

P	1.9205995	-0.7686107	-0.4465769
C	2.6737548	1.0051433	-0.2720766
C	2.7922867	1.3730365	1.2074174
C	1.6501834	1.6925343	1.9624075
C	4.0245931	1.3768854	1.8777033
C	1.7401916	2.0416827	3.3063267
H	0.6735487	1.6621930	1.4959246
C	4.1179201	1.7128078	3.2294613
H	4.9280471	1.1219648	1.3381379
C	2.9787360	2.0625857	3.9514882
H	0.8343073	2.2853268	3.8553896
H	5.0908670	1.7005643	3.7142414
H	3.0496989	2.3294266	5.0023654
C	4.0510498	1.0201151	-0.9780063
C	4.7968763	2.2097713	-0.9425718
C	4.5619307	-0.0508849	-1.7145863
C	6.0208507	2.3150274	-1.5962231
H	4.4070027	3.0636392	-0.3955580
C	5.7900356	0.0487775	-2.3749644
H	3.9912285	-0.9719167	-1.7810120
C	6.5279301	1.2285077	-2.3164463
H	6.5778893	3.2473272	-1.5492988
H	6.1657565	-0.8038766	-2.9347355
H	7.4833510	1.3069165	-2.8284174
C	1.8397706	2.0108401	-1.0877476
C	1.5526160	3.3015786	-0.6284523
C	1.4220465	1.6582742	-2.3790735
C	0.8230814	4.1954991	-1.4170395
H	1.8870196	3.6105167	0.3562500
C	0.6918118	2.5441028	-3.1650128
H	1.6602182	0.6634273	-2.7464905
C	0.3782879	3.8184438	-2.6834417
H	0.6021975	5.1886266	-1.0340034
H	0.3618712	2.2389663	-4.1545998
H	-0.1991674	4.5094881	-3.2915430
W	3.0825505	-2.5671318	1.1068788
C	3.4853420	-3.5648955	-0.6387883
O	3.6999583	-4.1304263	-1.6297172
C	4.9203717	-1.6438588	1.0335602
O	6.0128423	-1.2549511	1.0690374
C	4.0278786	-3.9420149	2.1990700
O	4.5856907	-4.7391774	2.8514642
C	2.5136722	-1.5542494	2.8135251
O	2.1580136	-1.0953419	3.8132750
C	1.4123411	-3.7214591	1.3986010
O	0.5382127	-4.4435628	1.6492048
C	0.1295868	-0.6694617	-0.2586337
C	-0.5434551	-1.9191119	-0.3427415
C	-0.7114065	0.4683613	-0.1947369
C	-1.9153840	-2.0315500	-0.2996940
H	0.0494375	-2.8203268	-0.4690397
C	-2.0908765	0.3607887	-0.1676502
H	-0.2850872	1.4622974	-0.1732303
C	-2.7600347	-0.8895456	-0.1990507
H	-2.3660140	-3.0167379	-0.3785870
H	-2.6795156	1.2701038	-0.0838774
C	-4.1952630	-0.9976671	-0.1403652
C	-4.8239489	-2.1971394	0.4060885
C	-6.0599449	-2.6760311	-0.0902517
C	-4.2273127	-2.9289333	1.4607095
C	-6.6577527	-3.8186516	0.4311755
H	-6.5381639	-2.1457038	-0.9087624
C	-4.8277615	-4.0699498	1.9821997
H	-3.2900037	-2.5748165	1.8793870
C	-6.0477037	-4.5274267	1.4720954
H	-7.6013038	-4.1661429	0.0174387
H	-4.3473673	-4.6017199	2.7997813
H	-6.5153359	-5.4194529	1.8794402
C	-5.0399230	0.0925321	-0.6222116
C	-4.6589893	0.8902787	-1.7273342
C	-6.2781207	0.3949645	-0.0072640
C	-5.4641791	1.9281389	-2.1847658
H	-3.7255235	0.6687335	-2.2361444
C	-7.0808054	1.4349060	-0.4643812
H	-6.5944189	-0.1902046	0.8514544
C	-6.6819978	2.2122078	-1.5574009
H	-5.1468888	2.5134030	-3.0443561
H	-8.0199139	1.6486256	0.0402036
H	-7.3098899	3.0235941	-1.9148413

4.xyz
79
Energy = -2442.096883176

P	1.8652947	-0.6364295	0.1204721
C	2.6463357	1.0894022	-0.1082861
C	2.8931899	1.5548245	1.3336304
C	1.8014424	1.9265573	2.1371931
C	4.1641869	1.5439621	1.9221636
C	1.9788591	2.3225680	3.4588973
H	0.7986385	1.9029689	1.7236456
C	4.3448835	1.9366736	3.2499167
H	5.0250491	1.2334216	1.3434877
C	3.2574212	2.3381898	4.0220745
H	1.1160901	2.6105865	4.0527401
H	5.3430876	1.9203440	3.6780737
H	3.3984315	2.6429305	5.0548625
C	3.9317452	0.9504180	-0.9489895
C	4.8348879	2.0236843	-0.9805172
C	4.1675096	-0.1361364	-1.7960306
C	5.9640553	1.9839841	-1.7940365
H	4.6464849	2.9010463	-0.3691407
C	5.2960863	-0.1793198	-2.6166964
H	3.4621168	-0.9623542	-1.8199352
C	6.2058517	0.8756264	-2.6106381
H	6.6532256	2.8238496	-1.7956773
H	5.4591585	-1.0407525	-3.2581132
H	7.0884484	0.8431973	-3.2429516
C	1.7656820	2.0361227	-0.9389244
C	1.5338348	3.3616875	-0.5593976
C	1.2524095	1.5889523	-2.1648634
C	0.7647901	4.2064129	-1.3646886
H	1.9463712	3.7399653	0.3696549
C	0.4830366	2.4265952	-2.9652592
H	1.4456247	0.5680221	-2.4826764
C	0.2266767	3.7406626	-2.5632327
H	0.5895860	5.2310930	-1.0487510
H	0.0805092	2.0534647	-3.9026732
H	-0.3784822	4.3955120	-3.1835391
W	3.1881977	-2.4751295	1.2653293
C	3.3085690	-3.5045491	-0.5166315
O	3.3727467	-4.0840722	-1.5150674
C	5.0068415	-1.5683552	0.9028753
O	6.0829031	-1.1652291	0.7799725
C	4.2631332	-3.8878324	2.2150777
O	4.8836371	-4.7010174	2.7677448
C	2.9777792	-1.4582257	3.0561345
O	2.8332143	-0.9658877	4.0884549
C	1.5330847	-3.5587803	1.8233832
O	0.6660009	-4.2206192	2.2098010
C	0.1292829	-0.6102814	0.0341453
C	-0.5144761	-1.8951728	-0.0141958
C	-0.7412623	0.5286269	-0.0192908
C	-1.8697781	-2.0312439	-0.0774250
H	0.1064611	-2.7836441	-0.0528873
C	-2.0981121	0.3909478	-0.0962321
H	-0.3285759	1.5262860	0.0368410
C	-2.7453427	-0.8914169	-0.1245123
H	-2.2965932	-3.0248910	-0.1607889
H	-2.7141812	1.2837898	-0.0712518
C	-4.1412411	-1.0194502	-0.1970572
C	-4.8148049	-2.2707228	0.1717224
C	-5.9231278	-2.7314454	-0.5681940
C	-4.3969402	-3.0268545	1.2859312
C	-6.5676462	-3.9155991	-0.2250056
H	-6.2589267	-2.1605959	-1.4287358
C	-5.0514986	-4.2042564	1.6352135
H	-3.5741389	-2.6630260	1.8938754
C	-6.1349401	-4.6575345	0.8779654
H	-7.4081347	-4.2631963	-0.8189514
H	-4.7237559	-4.7645963	2.5061750
H	-6.6435824	-5.5778248	1.1501123
C	-4.9866867	0.0927522	-0.6487493
C	-4.6001260	0.9156779	-1.7264349
C	-6.2280273	0.3455665	-0.0295561
C	-5.4144246	1.9600399	-2.1547455
H	-3.6698714	0.7049606	-2.2455390
C	-7.0343741	1.3978832	-0.4511816
H	-6.5419877	-0.2800398	0.8006124
C	-6.6314076	2.2102022	-1.5154035
H	-5.1061653	2.5731098	-2.9968750
H	-7.9786949	1.5876572	0.0510350
H	-7.2655441	3.0262576	-1.8494845

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79
Energy = -2441.916876646

P	1.8874958	-0.5824880	0.4419660
C	2.6079591	1.1184426	-0.0103537
C	3.0208320	1.6118189	1.3867279
C	2.0222264	1.9601146	2.3151505
C	4.3550544	1.6378040	1.8134602
C	2.3473222	2.3741967	3.6033847
H	0.9773417	1.9183227	2.0251432
C	4.6822269	2.0513263	3.1051372
H	5.1475587	1.3481126	1.1351024
C	3.6840748	2.4323852	4.0014158
H	1.5562602	2.6446486	4.2959581
H	5.7244879	2.0719047	3.4085153
H	3.9428018	2.7545563	5.0052496
C	3.7779267	0.9282553	-0.9904979
C	4.6716390	1.9924944	-1.1792512
C	3.9032779	-0.1989920	-1.8069115
C	5.6927572	1.9033034	-2.1214436
H	4.5612880	2.8991921	-0.5922696
C	4.9236677	-0.2916681	-2.7547554
H	3.1960452	-1.0193819	-1.7128820
C	5.8297741	0.7554390	-2.9070209
H	6.3791136	2.7355249	-2.2468823
H	5.0040821	-1.1817181	-3.3716605
H	6.6285163	0.6861047	-3.6392915
C	1.6084976	2.0213484	-0.7448378
C	1.3538477	3.3357825	-0.3426703
C	0.9876998	1.5384848	-1.9058078
C	0.4590978	4.1336375	-1.0609526
H	1.8487005	3.7443514	0.5315514
C	0.0936795	2.3299569	-2.6189695
H	1.2009043	0.5296532	-2.2489722
C	-0.1834466	3.6314096	-2.1916066
H	0.2696829	5.1510726	-0.7316627
H	-0.3857380	1.9313426	-3.5082623
H	-0.8824269	4.2520456	-2.7443432
W	3.1768869	-2.3984460	1.4522728
C	3.1184205	-3.4955952	-0.3052728
O	3.0883936	-4.1029357	-1.2830146
C	4.9910952	-1.5682722	0.8962990
O	6.0432309	-1.1786623	0.6375964
C	4.2297290	-3.9034892	2.3548619
O	4.8159526	-4.7537271	2.8680069
C	3.2531354	-1.3637879	3.2558628
O	3.2844581	-0.8441953	4.2792573
C	1.4598470	-3.3109640	2.1301770
O	0.5279130	-3.8426353	2.5536957
C	0.1186913	-0.6110363	0.2870521
C	-0.4653256	-1.8840202	0.0443632
C	-0.7485806	0.5084771	0.3790148
C	-1.8239226	-2.0271145	-0.1229390
H	0.1761078	-2.7508541	-0.0724872
C	-2.1066526	0.3646605	0.2122698
H	-0.3544573	1.4912251	0.5981836
C	-2.6906110	-0.9026292	-0.0578357
H	-2.2307076	-2.9988457	-0.3791852
H	-2.7504320	1.2285104	0.3353882
C	-4.1020951	-1.0343931	-0.2749037
C	-4.7808502	-2.2759129	0.0418446
C	-5.8774773	-2.7152143	-0.7373197
C	-4.3672640	-3.0684616	1.1392206
C	-6.5189956	-3.9093605	-0.4397353
H	-6.1832776	-2.1319192	-1.5995456
C	-5.0279541	-4.2502567	1.4433272
H	-3.5598387	-2.7175368	1.7737550
C	-6.0999523	-4.6772893	0.6520829
H	-7.3420314	-4.2495152	-1.0601417
H	-4.7188272	-4.8372409	2.3023623
H	-6.6099745	-5.6062731	0.8880498
C	-4.8565126	0.0780537	-0.8219342
C	-4.2724370	0.9539029	-1.7683087
C	-6.1948588	0.3053705	-0.4234351

C	-5.0007850	2.0124021	-2.2922810
H	-3.2634534	0.7609725	-2.1187673
C	-6.9096073	1.3790299	-0.9364021
H	-6.6429559	-0.3410374	0.3239535
C	-6.3175162	2.2323993	-1.8735948
H	-4.5516484	2.6628164	-3.0363546
H	-7.9266605	1.5591806	-0.6030715
H	-6.8824259	3.0658366	-2.2798244

5=.xyz
68
Energy = -1807.954440178

C	-5.5712789	2.7174408	-1.0823390
C	-4.5354834	2.1668985	-1.8568379
C	-3.8894573	0.9990464	-1.4779230
C	-4.2321634	0.2741341	-0.2898066
C	-5.2789179	0.8726713	0.4840176
C	-5.9177924	2.0454647	0.1006482
C	-3.5384731	-0.9277657	0.0857618
C	-4.0762902	-1.9004781	1.0007002
C	-5.4734515	-2.0806226	1.2567147
C	-5.9555993	-3.0480666	2.1301209
C	-5.0890050	-3.9104428	2.8200981
C	-3.7110422	-3.7685976	2.5825530
C	-3.2223792	-2.8078139	1.7083469
C	-2.2051530	-1.1874511	-0.4988714
C	-1.8569189	-2.4499057	-1.0335977
C	-0.6073539	-2.7054029	-1.5784903
C	0.4057229	-1.7135761	-1.6656223
C	0.0559394	-0.4522233	-1.1279568
C	-1.1942484	-0.2095622	-0.5628344
P	1.9507301	-2.2304870	-2.4737468
C	3.2199215	-0.7842935	-2.1967187
C	3.0633692	0.3509616	-3.2190176
C	4.1761306	1.0980380	-3.6355762
C	4.0462653	2.1408469	-4.5578309
C	2.7903827	2.4684876	-5.0701835
C	1.6716393	1.7390520	-4.6542993
C	1.8115808	0.6855764	-3.7484872
C	3.1754045	-0.2322261	-0.7659133
C	3.3338454	1.1316912	-0.4839651
C	3.2801162	1.6118610	0.8275359
C	3.0762350	0.7351315	1.8923895
C	2.9210053	-0.6280906	1.6265554
C	2.9637303	-1.0992974	0.3176717
C	4.5349637	-1.5256450	-2.4668957
C	5.5023972	-1.7914388	-1.4908214
C	6.6684854	-2.4960927	-1.8042793
C	6.8911864	-2.9541109	-3.1047480
C	5.9374214	-2.6871999	-4.0918423
C	4.7818892	-1.9741991	-3.7785773
H	3.4805992	1.8342011	-1.2980192
H	2.7961901	-2.1505820	0.0976293
H	3.3929843	2.6779010	1.0121840
H	2.7424346	-1.3251483	2.4419801
H	3.0227681	1.1086693	2.9121458
H	5.3458183	-1.4434231	-0.4747587
H	4.0441093	-1.7603310	-4.5467578
H	7.4046303	-2.6853790	-1.0261556
H	6.0986192	-3.0299096	-5.1115430
H	7.7972587	-3.5034774	-3.3482315
H	5.1574068	0.8537481	-3.2376152
H	0.9488110	0.0967053	-3.4523709
H	4.9275167	2.6940289	-4.8752825
H	0.6866713	1.9843025	-5.0448811
H	2.6835711	3.2776139	-5.7888365
H	-0.3950255	-3.7035571	-1.9666476
H	0.7814728	0.3545693	-1.1302869
H	-2.5957771	-3.2495869	-1.0003289
H	-1.3993326	0.7778059	-0.1527467
H	-6.1879771	-1.4653881	0.7181736
H	-2.1497826	-2.7266222	1.5561540
H	-7.0328725	-3.1427064	2.2663454
H	-3.0047128	-4.4172691	3.1003392
H	-5.4694769	-4.6619680	3.5070961
H	-3.0900047	0.6117177	-2.1030267
H	-5.5610769	0.4139499	1.4268457
H	-4.2323915	2.6594654	-2.7805876
H	-6.6964328	2.4534977	0.7451556
H	-6.0774607	3.6314330	-1.3821252

5•-.xyz
68
Energy = -1807.891691468

P	1.8448419	-0.4839441	-1.2466514
C	2.4978382	1.2909263	-0.8096099
C	2.0114556	1.7419362	0.5720135
C	1.5581233	3.0439843	0.8192052
C	2.0081034	0.8337179	1.6426261
C	1.1047885	3.4224268	2.0861330
H	1.5375171	3.7682891	0.0115689
C	1.5651497	1.2081610	2.9075497
H	2.3350387	-0.1859031	1.4571235
C	1.1046717	2.5077324	3.1375530
H	0.7459343	4.4364308	2.2445403
H	1.5650510	0.4788945	3.7137680
H	0.7432917	2.7980509	4.1206319
C	4.0201465	1.0665511	-0.8216317
C	4.8415762	1.2449445	0.2963290
C	4.6231095	0.6730541	-2.0293706
C	6.2205842	1.0257014	0.2166966
H	4.4060222	1.5628443	1.2378384
C	5.9948113	0.4486125	-2.1111534
H	3.9977725	0.5463937	-2.9091889
C	6.8043651	0.6229360	-0.9840409
H	6.8373583	1.1756146	1.0994869
H	6.4348233	0.1409246	-3.0565039
H	7.8759535	0.4522135	-1.0452236
C	2.1493254	2.3307051	-1.8865662
C	2.9908984	3.4346769	-2.0939580
C	0.9880988	2.2346143	-2.6607487
C	2.6825323	4.4111020	-3.0420409
H	3.9002091	3.5268093	-1.5064770
C	0.6708272	3.2117428	-3.6066148
H	0.3347769	1.3787526	-2.5252958
C	1.5174759	4.3042214	-3.8045003
H	3.3542590	5.2538908	-3.1859010
H	-0.2378070	3.1133222	-4.1954322
H	1.2758676	5.0600099	-4.5473976
C	0.1205390	-0.5438488	-0.7930458
C	-0.5024363	-1.8231324	-0.9222517
C	-0.7314200	0.5005124	-0.3374317
C	-1.8309024	-2.0359408	-0.6298399
H	0.0990571	-2.6601953	-1.2778507
C	-2.0661698	0.2891325	-0.0548650
H	-0.3261617	1.4944154	-0.1862115
C	-2.6885618	-0.9848308	-0.1831819
H	-2.2489072	-3.0296639	-0.7684118
H	-2.6573772	1.1223697	0.3151231
C	-4.0774681	-1.1994848	0.1178378
C	-4.5497508	-2.5158656	0.5385082
C	-5.8383468	-2.9919628	0.1913117
C	-3.7455659	-3.3797453	1.3224560
C	-6.2882610	-4.2450219	0.5943358
H	-6.4814908	-2.3631954	-0.4182511
C	-4.1959099	-4.6329810	1.7245156
H	-2.7609260	-3.0384418	1.6286668
C	-5.4721954	-5.0819361	1.3647944
H	-7.2799578	-4.5784444	0.2965259
H	-3.5517889	-5.2616872	2.3353950
H	-5.8237974	-6.0606452	1.6797043
C	-5.0385917	-0.1054423	0.0159679
C	-4.9045178	0.9195003	-0.9532156
C	-6.1592191	-0.0167470	0.8787219
C	-5.8216698	1.9606111	-1.0483715
H	-4.0698977	0.8747643	-1.6467694
C	-7.0768434	1.0238236	0.7819118
H	-6.2913291	-0.7765747	1.6439496
C	-6.9191257	2.0267613	-0.1820504
H	-5.6883154	2.7221328	-1.8136214
H	-7.9176444	1.0611919	1.4712094
H	-7.6359439	2.8399303	-0.2573978

5.xyz
68
Energy = -1807.782810504

P	1.8659371	-0.6698072	-0.3913296
C	2.5966415	1.1044797	-0.3836193
C	2.6611498	1.3706287	1.1259612
C	1.5579570	1.8743596	1.8359418
C	3.7979845	0.9979623	1.8629044
C	1.6000930	2.0274829	3.2192825
H	0.6526677	2.1441589	1.3050301
C	3.8405871	1.1465107	3.2491027
H	4.6583319	0.5868419	1.3450704
C	2.7439421	1.6674948	3.9362658
H	0.7335495	2.4265678	3.7395168
H	4.7350007	0.8513167	3.7910700
H	2.7763531	1.7874454	5.0154330
C	4.0062886	1.0694963	-1.0114815
C	4.8423100	2.1808560	-0.8206427
C	4.4609306	0.0296294	-1.8251685
C	6.0995548	2.2425225	-1.4133743
H	4.4997360	3.0034192	-0.1989957
C	5.7226903	0.0883710	-2.4263925
H	3.8280511	-0.8363820	-2.0011550
C	6.5478929	1.1917484	-2.2208150
H	6.7302347	3.1122206	-1.2497737
H	6.0544576	-0.7335070	-3.0550476
H	7.5287556	1.2381994	-2.6856789
C	1.8283760	2.1346375	-1.2147756
C	1.6504180	3.4568448	-0.7919919
C	1.3730424	1.7766253	-2.4918624
C	0.9932999	4.3835120	-1.6053955
H	2.0199221	3.7686790	0.1794726
C	0.7199588	2.6974611	-3.3053225
H	1.5201727	0.7564234	-2.8379920
C	0.5176654	4.0071959	-2.8609279
H	0.8568698	5.4023166	-1.2526585
H	0.3641421	2.3928866	-4.2857286
H	0.0002317	4.7261368	-3.4897935
C	0.1343414	-0.5754251	-0.3142629
C	-0.5059093	-1.8654281	-0.1976782
C	-0.7523182	0.5548482	-0.3530851
C	-1.8588130	-2.0091761	-0.1170495
H	0.1256450	-2.7517973	-0.1862880
C	-2.1082831	0.4090785	-0.3050532
H	-0.3417662	1.5529472	-0.4264758
C	-2.7466445	-0.8753355	-0.1798094
H	-2.2852412	-3.0051180	-0.0585462
H	-2.7311259	1.2978207	-0.3095213
C	-4.1398822	-1.0062501	-0.1221355
C	-4.7786739	-2.2297256	0.3860681
C	-5.9334462	-2.7456534	-0.2359728
C	-4.2826699	-2.8966212	1.5240707
C	-6.5487851	-3.8984629	0.2429198
H	-6.3326008	-2.2416253	-1.1112247
C	-4.9069322	-4.0422071	2.0098915
H	-3.4196202	-2.4887424	2.0416582
C	-6.0386576	-4.5523679	1.3681500
H	-7.4278499	-4.2892249	-0.2619055
H	-4.5162415	-4.5325958	2.8971044
H	-6.5241156	-5.4473383	1.7466383
C	-5.0328727	0.0720484	-0.5724217
C	-4.7599272	0.8100523	-1.7417918
C	-6.2112641	0.3704968	0.1412132
C	-5.6199690	1.8184330	-2.1681257
H	-3.8809463	0.5619255	-2.3292067
C	-7.0641613	1.3862732	-0.2798862
H	-6.4406714	-0.1918899	1.0414982
C	-6.7725083	2.1157649	-1.4363027
H	-5.3983230	2.3657016	-3.0800890
H	-7.9582378	1.6116178	0.2946549
H	-7.4428308	2.9029404	-1.7692384

5•+.xyz
68
Energy = -1807.603169365

P	1.7462582	-0.3600295	-1.3609348
C	2.4704628	1.3272477	-0.8349576
C	1.9546977	1.7331811	0.5426847
C	1.4640214	3.0166430	0.8031929
C	1.9513181	0.7893179	1.5817898
C	0.9613286	3.3427558	2.0656472
H	1.4607146	3.7616088	0.0141343
C	1.4480544	1.1106281	2.8391071
H	2.3479084	-0.2078827	1.4013923
C	0.9447475	2.3910582	3.0848682
H	0.5793456	4.3432285	2.2474937
H	1.4492599	0.3631979	3.6271033
H	0.5482603	2.6437583	4.0637795
C	3.9873001	1.0262872	-0.8180348
C	4.7912261	1.2664510	0.2999114
C	4.5882785	0.5326235	-1.9866781
C	6.1656150	1.0158336	0.2514130
H	4.3530934	1.6630829	1.2091234
C	5.9559955	0.2781930	-2.0350729
H	3.9805549	0.3609345	-2.8724313
C	6.7517641	0.5177441	-0.9109894
H	6.7755750	1.2161507	1.1276826
H	6.4006894	-0.1036308	-2.9494648
H	7.8192113	0.3202728	-0.9450988
C	2.1735893	2.3784744	-1.9154941
C	3.0832448	3.4248700	-2.1248129
C	0.9991104	2.3531068	-2.6771781
C	2.8147856	4.4259223	-3.0559645
H	4.0039328	3.4568957	-1.5506366
C	0.7335877	3.3485221	-3.6202572
H	0.2790441	1.5511949	-2.5451714
C	1.6386620	4.3909016	-3.8101993
H	3.5277164	5.2335309	-3.1952064
H	-0.1793649	3.3027701	-4.2069018
H	1.4353309	5.1663863	-4.5427568
C	0.0393919	-0.4464555	-0.8467537

C -0.5431002 -1.7309765 -1.0426223
C -0.7852550 0.5836517 -0.3208661
C -1.8586515 -1.9797845 -0.7153988
H 0.0635537 -2.5270983 -1.4664475
C -2.1094213 0.3467502 -0.0306524
H -0.3690027 1.5649380 -0.1315052
C -2.6851260 -0.9426597 -0.2059235
H -2.2866042 -2.9584342 -0.9029639
H -2.7154432 1.1391238 0.3960928
C -4.0613419 -1.1840499 0.1265952
C -4.4875984 -2.4941815 0.5708743
C -5.7814225 -2.9739215 0.2519023
C -3.6267887 -3.3144906 1.3402569
C -6.1864689 -4.2324795 0.6715409
H -6.4341513 -2.3685316 -0.3679535
C -4.0495363 -4.5609438 1.7772632
H -2.6516346 -2.9381041 1.6309821
C -5.3257556 -5.0254407 1.4387468
H -7.1687373 -4.6035392 0.3976200
H -3.3931301 -5.1705169 2.3897001
H -5.6501942 -6.0054441 1.7749777
C -5.0322099 -0.1135749 0.0233684
C -4.9219730 0.8678147 -0.9915520
C -6.1130084 -0.0338188 0.9343642
C -5.8610845 1.8836015 -1.0913036
H -4.1266927 0.7849311 -1.7252201
C -7.0331197 1.0006477 0.8429085
H -6.1857949 -0.7600968 1.7369799
C -6.9130609 1.9571522 -0.1710181
H -5.7859157 2.6148224 -1.8897066
H -7.8413702 1.0702662 1.5636483
H -7.6407773 2.7593110 -0.2460913

DbuH$^+$.xyz
28
Energy = -462.8512737218
C -1.9801291 -1.3400915 -0.3387410
C -0.8500938 -1.4505134 0.7121373
C 0.3854802 -0.6970263 0.3176588
C -2.7731577 -0.0320242 -0.2541470
C -1.9431404 1.2406108 -0.4560935
C -0.8235525 1.4211629 0.5748825
H -2.6615778 -2.1799980 -0.1714013
H -1.2028897 -1.0805652 1.6818248
H -3.5764082 -0.0569368 -0.9986303
H -1.5093893 1.2686403 -1.4635081
H -1.5547685 -1.4705528 -1.3413704
H -0.5694049 -2.4979166 0.8492112
H -3.2574442 0.0200761 0.7306721
H -2.6052517 2.1094210 -0.3708135
H -1.1732185 1.1684722 1.5820202
H -0.4917977 2.4597584 0.5956135
N 0.3937285 0.6286250 0.2778102
C 1.6022642 1.3720523 -0.1445202
C 2.8601557 0.5649944 0.1504916
H 1.5165549 1.6037481 -1.2123634
H 1.6069439 2.3127283 0.4090949
C 2.7380338 -0.8278797 -0.4531448
H 3.7270201 1.0789498 -0.2703945
H 3.0017902 0.4870999 1.2330924
H 2.7723292 -0.7931924 -1.5473514
H 3.5319122 -1.4899717 -0.1035202
N 1.4559782 -1.4064331 -0.0298172
H 1.3800321 -2.4132380 0.0413065

Dbu.xyz
27
Energy = -462.3785275343
C -1.9457805 -1.3873912 -0.2941679
C -0.8390877 -1.4892307 0.7788912
C 0.4573136 -0.8294755 0.3638199
C -2.6977936 -0.0510350 -0.2994396
C -1.8173098 1.1848514 -0.5174303
C -0.7288481 1.3537464 0.5553757
H -2.6701126 -2.1913177 -0.1172033
H -1.2054599 -1.0704681 1.7257100
H -3.4776022 -0.0804633 -1.0706211
H -1.3398031 1.1508919 -1.5055216
H -1.4994551 -1.5758810 -1.2795323
H -0.5927319 -2.5389696 0.9522049
H -3.2144166 0.0616502 0.6650446
H -2.4550936 2.0777131 -0.5000781
H -1.1499868 1.1371957 1.5461969
H -0.3906622 2.3931475 0.5758142
N 0.4754646 0.5451586 0.3369001
C 1.6716418 1.2485048 -0.1382456
C 2.9087036 0.4052440 0.1445274
H 1.5900846 1.4604286 -1.2152762
H 1.7247909 2.2097361 0.3839609
C 2.6901322 -0.9998048 -0.4163013
H 3.7916172 0.8768718 -0.3002616
H 3.0669626 0.3470781 1.2282678
H 2.6899759 -0.9640667 -1.5167680
H 3.5173570 -1.6589307 -0.1272735
N 1.4400992 -1.6151842 0.0414063

Et_3NHCl.xyz
24
Energy = -753.4825987280
N 0.3583753 -0.0023598 0.1467380
C 0.1176199 1.2356261 0.9756902
C 0.4647170 2.5201663 0.2374759
H 0.7541001 1.1154491 1.8554113
H -0.9249258 1.2169837 1.3028700
H 0.4204535 3.3488779 0.9499457
H 1.4785476 2.4689069 -0.1707525
H -0.2385185 2.7374311 -0.5711147
C 0.0964358 -1.2328077 0.9804582
C 0.4205021 -2.5259831 0.2468895
H -0.9454345 -1.1947033 1.3081554
H 0.7354351 -1.1204838 1.8593880
H 0.3601915 -3.3513560 0.9620528
H -0.2858036 -2.7329203 -0.5617318
H 1.4355153 -2.4947748 -0.1603744
C -0.3513106 0.0011550 -1.1831362
C -1.8681911 0.0116931 -1.0722495
H 0.0052417 -0.8801888 -1.7176747
H 0.0172998 0.8764906 -1.7193767
H -2.2873940 0.0144457 -2.0822403
H -2.2479034 -0.8743205 -0.5552594
H -2.2355911 0.9030233 -0.5555032
H 1.4147669 -0.0118165 -0.0773249
Cl 3.3058716 -0.0285346 -0.3983369

Et_3NH^+.xyz
23
Energy = -293.0494488383
N 0.0085171 -0.1287459 -0.5034667
C 1.2109469 -1.0090931 -0.2021421
C 2.5320097 -0.3403106 -0.5408264
H 1.0596197 -1.9113875 -0.7972623
H 1.1398536 -1.2768916 0.8530485
H 3.3256567 -1.0844274 -0.4320547
H 2.5453298 0.0164040 -1.5758323
H 2.7621082 0.4925205 0.1280713
C -1.2740717 -0.9107807 -0.2686299
C -2.5180695 -0.1413610 -0.6781650
H -1.2816540 -1.1795932 0.7886680
H -1.1621510 -1.8243509 -0.8552639
H -3.3726286 -0.8202170 -0.6127141
H -2.7175318 0.7096681 -0.0224844
H -2.4472955 0.2111532 -1.7122901
C 0.0429163 1.2177588 0.2072339
C -0.0033194 1.1027729 1.7203945
H -0.8059377 1.7807980 -0.1817422
H 0.9542380 1.7101006 -0.1332840
H 0.0261418 2.1156397 2.1308455
H -0.9231395 0.6284656 2.0724623
H 0.8547301 0.5569112 2.1213494
H 0.0437309 0.0849659 -1.5059149

Et_3N.xyz
22
Energy = -292.5917896525
N -0.1538466 -0.5408926 -0.0001190
C -0.9472155 -0.2502161 1.2049316
C -0.2708968 -0.7015845 2.4980060
H -1.8943470 -0.7901560 1.0873365
H -1.2072721 0.8231993 1.2789101
H -0.9743591 -0.6101017 3.3323709
H 0.0433156 -1.7483029 2.4216755
H 0.6075784 -0.0943700 2.7388505
C -0.9471764 -0.2503587 -1.2052151
C -0.2709939 -0.7021647 -2.4982107
H -1.2070613 0.8230800 -1.2794634
H -1.8943963 -0.7901187 -1.0874814
H -0.9744095 -0.6105513 -3.3326012
H 0.6077076 -0.0953125 -2.7391343
H 0.0428185 -1.7489858 -2.4217056
C 1.1746229 0.1000655 -0.0001347
C 1.1961921 1.6378838 0.0005787
H 1.7161311 -0.2705238 -0.8760062
H 1.7165492 -0.2713361 0.8751365
H 2.2331843 1.9914436 0.0001406
H 0.7014213 2.0500850 -0.8853556
H 0.7024528 2.0492181 0.8874903

Fc.xyz
21
Energy = -1651.176075694
Fe -0.0001423 -0.0018492 0.0001852
C -0.0005093 1.2195924 1.6286845
C 0.0012801 1.2194796 -1.6286656
C 0.7161918 -0.9863753 1.6323956
C -0.7167812 -0.9859436 -1.6324736
C 0.7166165 -0.9868515 -1.6316670
C -0.7172139 -0.9863380 1.6319561
C 1.1605099 0.3761497 -1.6294024
C -1.1602593 0.3769688 1.6296188
C 1.1591731 0.3768963 1.6303595
C -1.1589229 0.3775719 -1.6306721
H -0.0003396 2.3012613 1.6011517
H 0.0017879 2.3011710 -1.6013481
H 1.3518963 -1.8616388 1.6084827
H -1.3530605 -1.8608096 -1.6088505
H 1.3520870 -1.8622978 -1.6073344
H -1.3532154 -1.8613867 1.6077703
H 2.1894534 0.7098586 -1.6029630
H -2.1889902 0.7113465 1.6033813
H 2.1880234 0.7109516 1.6044747
H -2.1875848 0.7122428 -1.6050838

Fc$^{\bullet+}$.xyz
21
Energy = -1650.991171119
Fe 0.0000039 -0.0000002 -0.1091508
C -0.0001392 -1.7628966 -1.3154229
C 0.0001387 1.7628968 -1.3154227
C 0.7181314 -1.6499381 0.8782758
C -0.7181316 1.6499478 0.8782745
C 0.7180110 1.6499565 0.8783959
C -0.7180114 -1.6499668 0.8783942
C 1.1535856 1.7179115 -0.4834320
C -1.1535837 -1.7179296 -0.4834309
C 1.1534692 -1.7178499 -0.4836464
C -1.1534673 1.7178682 -0.4836448
H -0.0002139 -1.7639864 -2.3973449
H 0.0002098 1.7639873 -2.3973446
H 1.3570183 -1.5990417 1.7490037
H -1.3570211 1.5990530 1.7490007
H 1.3568521 1.5990280 1.7491663
H -1.3568545 -1.5990395 1.7491632
H 2.1797947 1.6973503 -0.8245359
H -2.1797933 -1.6973734 -0.8245337
H 2.1796574 -1.6973083 -0.8248059
H -2.1796561 1.6973311 -0.8248038

$Li(Thf)_4^+$.xyz
53
Energy = -937.8922315317
Li -0.3878473 -0.0917393 -0.0809383
O 0.6330234 1.0815288 1.0784225
O 0.8202987 -0.9439464 -1.3200077
O -1.7122103 0.9779662 -0.9960052
O -1.2138970 -1.4434329 1.0167280
C 1.2621179 2.2957956 0.5696049
C 0.4841093 1.1764736 2.5296450
C 0.3785807 -2.0400733 -2.1828834
C 2.2466918 -1.0829606 -1.0491442
C -2.4983323 2.0059639 -0.3277254
C -1.7130800 1.2229460 -2.4391322
C -2.5771940 -1.3921358 1.5395822
C -0.4724451 -2.5121753 1.6762321
C 1.0880281 3.3256272 1.6776201
H 0.7649491 2.5538312 -0.3688428
H 2.3200022 2.0842350 0.3727529
C 1.2157256 2.4538485 2.9369253
H -0.5868575 1.2258825 2.7565229
H 0.9054700 0.2700127 2.9716823
C 1.6358791 -2.8445557 -2.5165346
H -0.3556556 -2.6275017 -1.6207547
H -0.1037445 -1.6060734 -3.0627602
C 2.5551145 -2.5485038 -1.3207873
H 2.7979086 -0.4190611 -1.7265913
H 2.4129230 -0.7676249 -0.0166638
C -2.5395857 3.1676284 -1.3104691
H -2.0020380 2.2328621 0.6189178
H -3.5010027 1.6089503 -0.1262688
C -2.6254790 2.4307147 -2.6566719
H -0.6791422 1.4214225 -2.7408616
H -2.0679150 0.3160236 -2.9357899
C -2.7347471 -2.6493988 2.3895784
H -2.6777106 -0.4793967 2.1390961
H -3.2584639 -1.3428127 0.6868149

C	-1.3032711	-2.8793151	2.8995263
H	0.5243612	-2.1301535	1.9117178
H	-0.3827829	-3.3527870	0.9775849
H	0.0935274	3.7818473	1.6241208
H	1.8379404	4.1184509	1.6278746
H	0.7732518	2.9126841	3.8239570
H	2.2694383	2.2414866	3.1443668
H	1.4189107	-3.9082636	-2.6382362
H	2.0904756	-2.4764989	-3.4417605
H	2.2773324	-3.1624618	-0.4572491
H	3.6115603	-2.7168218	-1.5430645
H	-1.6156836	3.7531051	-1.2484636
H	-3.3873687	3.8334561	-1.1329126
H	-2.2988735	3.0413322	-3.5013918
H	-3.6537746	2.1045801	-2.8422763
H	-3.4602220	-2.5119080	3.1946384
H	-3.0575192	-3.4921013	1.7695134
H	-1.0789408	-2.2021833	3.7306508
H	-1.1240825	-3.9057918	3.2276272

Ph_3C^-.xyz
34
Energy = -733.5893099198

C	0.0000225	0.0007612	0.0002376
C	0.0000460	-1.4517297	0.0002050
C	-1.0437887	-2.2167407	0.5952130
C	1.0438344	-2.2167206	-0.5949090
C	-1.0446030	-3.6068793	0.5924854
H	-1.8612850	-1.6903494	1.0805054
C	1.0444928	-3.6068602	-0.5924910
H	1.8614320	-1.6903189	-1.0800179
C	-0.0000878	-4.3305340	-0.0000675
H	-1.8651945	-4.1371685	1.0736490
H	1.8649672	-4.1371320	-1.0738745
H	-0.0000888	-5.4172834	-0.0001359
C	1.2579393	0.7266822	0.0005240
C	1.3986109	2.0146463	-0.5915088
C	2.4428575	0.2032194	0.5929776
C	2.6026599	2.7094933	-0.5888868
H	0.5337630	2.4612680	-1.0746898
C	3.6476002	0.8967709	0.5903328
H	2.3958053	-0.7690575	1.0760496
C	3.7521455	2.1645558	0.0006826
H	2.6515950	3.6863755	-1.0678394
H	4.5174274	0.4495713	1.0694059
H	4.6936890	2.7072535	0.0006203
C	-1.2579851	0.7265936	-0.0001868
C	-2.4427191	0.2031621	-0.5930041
C	-1.3988056	2.0144482	0.5919483
C	-3.6474277	0.8967775	-0.5907181
H	-2.3955478	-0.7691075	-1.0760825
C	-2.6027499	2.7094450	0.5888421
H	-0.5340775	2.4609526	1.0754514
C	-3.7520712	2.1645477	-0.0010521
H	-4.5171231	0.4496675	-1.0701136
H	-2.6517648	3.6863570	1.0677176
H	-4.6935683	2.7073317	-0.0012696

$Ph_3C^{\bullet}$.xyz
34
Energy = -733.4910097997

C	0.0000324	0.0002250	0.0001389
C	0.0000448	-1.4571987	0.0001386
C	-1.0173024	-2.1917596	0.6539890
C	1.0173544	-2.1917689	-0.6537561
C	-1.0133765	-3.5821622	0.6566012
H	-1.7986995	-1.6542578	1.1826410
C	1.0132586	-3.5821725	-0.6566051
H	1.7988591	-1.6542743	-1.1822568
C	-0.0001103	-4.2885002	-0.0000751
H	-1.7989493	-4.1199690	1.1806418
H	1.7987531	-4.1199856	-1.1807567
H	-0.0001793	-5.3747115	-0.0001882
C	1.2621688	0.7288942	0.0002778
C	1.3897335	1.9773282	-0.6534223
C	2.4070113	0.2149311	0.6539537
C	2.5960731	2.6687064	-0.6565276
H	0.5334589	2.3856731	-1.1816590
C	3.6093399	0.9132403	0.6563287
H	2.3320474	-0.7304182	1.1827580
C	3.7145075	2.1439732	-0.0002826
H	2.6691997	3.6178253	-1.1807337
H	4.4678878	0.5016274	1.1801943
H	4.6553286	2.6868406	-0.0005162
C	-1.2621564	0.7288266	-0.0000699
C	-2.4068755	0.2148713	-0.6539614
C	-1.3898515	1.9772103	0.6536623
C	-3.6091797	0.9132187	-0.6565992
H	-2.3318393	-0.7305218	-1.1826775
C	-2.5961445	2.6686572	0.6564757
H	-0.5337093	2.3854448	1.1821946
C	-3.7144612	2.1439284	0.0000417
H	-4.4676046	0.5016750	-1.1807213
H	-2.6693292	3.6178182	1.1805943
H	-4.6552903	2.6867839	0.0001773

Ph_3C^+.xyz
34
Energy = -733.3236384946

C	-0.0000025	-0.0000217	-0.0000142
C	-0.0000087	-1.4431128	-0.0000175
C	-1.0297205	-2.1632424	0.6563158
C	1.0297026	-2.1632512	-0.6563431
C	-1.0171930	-3.5493410	0.6653333
H	-1.7939250	-1.6197262	1.2013825
C	1.0172067	-3.5493507	-0.6652918
H	1.7938699	-1.6197442	-1.2014729
C	0.0000234	-4.2437630	0.0000520
H	-1.7908588	-4.0944622	1.1958849
H	1.7908619	-4.0944815	-1.1958494
H	0.0000704	-5.3294728	0.0001168
C	1.2497425	0.7215277	0.0000277
C	1.3585741	1.9731665	-0.6566928
C	2.3881803	0.1900947	0.6566884
C	2.5652548	2.6553461	-0.6658607
H	0.5058382	2.3630636	-1.2020094
C	3.5823417	0.8939619	0.6655612
H	2.2994498	-0.7431792	1.2022548
C	3.6751894	2.1218346	-0.0002662
H	2.6505837	3.5977015	-1.1967754
H	4.4411559	0.4967746	1.1964711
H	4.6154597	2.6646495	-0.0004354
C	-1.2497441	0.7215346	-0.0000583
C	-2.3881730	0.1901326	-0.6567530
C	-1.3585890	1.9731519	0.6566870
C	-3.5823391	0.8939921	-0.6655924
H	-2.2994279	-0.7431011	-1.2023828
C	-2.5652630	2.6553331	0.6658949
H	-0.5058561	2.3630095	1.2020313
C	-3.6751970	2.1218343	0.0002902
H	-4.4411494	0.4968222	-1.1965218
H	-2.6505900	3.5976705	1.1968409
H	-4.6154681	2.6646482	0.0005037

s2NH.xyz
28
Energy = -874.2191836246

H	-0.0001092	-0.0000456	-1.8270438
N	0.0000372	-0.0000117	-0.8099658
Si	-0.0035832	1.5880481	-0.0939440
Si	0.0035944	-1.5880557	-0.0939057
C	-1.7264994	2.0851979	0.4882886
C	1.1551884	1.6199828	1.3904941
C	0.5795639	2.8048447	-1.4050895
C	-1.1551552	-1.6199769	1.3905473
C	-0.5795782	-2.8048475	-1.4050451
C	1.7265077	-2.0852152	0.4883407
H	-1.7246701	3.0933841	0.9231254
H	1.1515761	2.6118614	1.8604975
H	-2.4376324	2.0778552	-0.3471639
H	2.1846664	1.3880165	1.0926270
H	0.8558892	0.8937204	2.1563328
H	-2.1007462	1.3913044	1.2509776
H	-0.0718157	2.7749694	-2.2880231
H	1.6015382	2.5759292	-1.7311191
H	0.5694676	3.8322565	-1.0197723
H	2.4377517	-2.0775132	-0.3470227
H	-2.1846028	-1.3877509	1.0927444
H	-1.6014914	-2.5758269	-1.7311584
H	0.0718223	-2.7749894	-2.2879537
H	-0.8556794	-0.8938729	2.1564789
H	2.1005304	-1.3915466	1.2513609
H	1.7247453	-3.0935543	0.9228090
H	-1.1517073	-2.6119104	1.8604384
H	-0.5696081	-3.8322533	-1.0197068

s2N$^-$.xyz
27
Energy = -873.6285660112

N	0.0000000	0.0000000	0.6567512
Si	0.4934735	-1.5012804	0.1876668
Si	-0.4934735	1.5012804	0.1876668
C	2.1305866	-1.5470967	-0.8108355
C	0.8103618	-2.6500031	1.6835886
C	-0.7492417	-2.4687834	-0.9078344
C	-2.1305866	1.5470967	-0.8108355
C	-0.8103618	2.6500031	1.6835886
C	0.7492417	2.4687834	-0.9078344
H	2.4471065	-2.5696629	-1.0672815
H	1.1430428	-3.6550472	1.3843841
H	2.0250254	-0.9830956	-1.7477644
H	-0.1041450	-2.7599735	2.2818367
H	1.5791348	-2.2201268	2.3397725
H	2.9413210	-1.0760076	-0.2387793
H	-0.9307062	-1.9320919	-1.8491929
H	-1.7171514	-2.5636487	-0.3973382
H	-0.3989861	-3.4812983	-1.1601624
H	1.7171514	2.5636487	-0.3973382
H	-2.9413210	1.0760076	-0.2387793
H	-1.5791348	2.2201268	2.3397725
H	0.1041450	2.7599735	2.2818367
H	-2.0250254	0.9830956	-1.7477644
H	0.9307062	1.9320919	-1.8491929
H	0.3989861	3.4812983	-1.1601624
H	-2.4471065	2.5696629	-1.0672815
H	-1.1430428	3.6550472	1.3843841

THF.xyz
13
Energy = -232.5925768658

O	-0.0245054	0.0050796	-1.2566000
C	0.1574203	1.1732744	-0.4160198
C	-0.1578689	-1.1733332	-0.4189083
C	0.2205287	-0.7343192	0.9959995
C	-0.2233095	0.7365449	0.9975554
H	1.2095905	1.4879507	-0.4657510
H	-0.4719515	1.9760648	-0.8126146
H	-1.1992148	-1.5208496	-0.4653973
H	0.4946778	-1.9544641	-0.8220144
H	-0.2721629	-1.3358687	1.7646850
H	1.3043227	-0.8033763	1.1415817
H	-1.3073581	0.8073848	1.1408167
H	0.2698311	1.3359120	1.7677406

VIa=.xyz
81
Energy = -1778.264235789

C	2.0287136	2.0997150	-0.3519547
C	2.6090086	1.5610541	0.7940654
C	3.4949426	0.4785730	0.7656141
C	3.8092471	-0.1440460	-0.4881744
C	3.3213026	0.4879610	-1.6754345
C	2.4329977	1.5699569	-1.5702435
P	4.6883187	-1.8084354	-0.5595656
C	3.2483122	-2.9033100	-0.5118411
C	3.4510756	-4.3040622	-0.6336372
C	2.3997454	-5.2115519	-0.6270062
C	1.0522500	-4.8086521	-0.4920860
C	0.8511854	-3.4216360	-0.3525061
C	1.8962251	-2.5022580	-0.3670520
C	-0.0682260	-5.7800809	-0.5161071
C	-1.1788804	-5.5088415	-1.3872783
C	-1.0578504	-4.5982616	-2.4892124
C	-2.1137890	-4.3024715	-3.3381581
C	-3.3833345	-4.8803025	-3.1612294
C	-3.5454092	-5.7570251	-2.0765025
C	-2.4914725	-6.0621340	-1.2234224
C	4.0843008	0.0387634	2.1333203
C	3.7290869	1.0215149	3.2717801
C	3.7218372	0.0763563	-3.1191224
C	3.2107779	1.0771609	-4.1804334
C	1.0101069	3.2379400	-0.2321312
C	1.6655218	4.4512689	0.4636268
C	0.0216089	-6.9374872	0.3288408
C	-0.6961832	-8.1607798	0.1132108
C	-0.5624206	-9.2648891	0.9459746
C	0.2904571	-9.2464095	2.0618477
C	1.0241913	-8.0690413	2.2921748
C	0.9026853	-6.9643876	1.4615780
C	3.5404056	-1.3388834	2.5708108
C	5.6275803	0.0183920	2.0652477
C	0.4789055	3.6950851	-1.6004063
C	-0.1882198	2.7567717	0.6160849
C	5.2605879	0.0716023	-3.2564642
C	3.1375880	-1.2975854	-3.5146161
H	4.4707366	-4.6761603	-0.7522799
H	1.6660685	-1.4453093	-0.2613686
H	2.6149115	-6.2749743	-0.7313382
H	-0.1683862	-3.0551502	-0.2397485
H	-1.3393748	-8.2453839	-0.7574646
H	1.4897520	-6.0751038	1.6734541
H	-1.1269809	-10.1680758	0.7134878
H	1.7004624	-8.0133933	3.1452721
H	0.3857385	-10.1098646	2.7152051

H	-0.0971126	-4.1197232	-2.6552488
H	-2.6847770	-6.7137316	-0.3766091
H	-1.9467781	-3.6081263	-4.1615059
H	-4.5215073	-6.2028573	-1.8840186
H	-4.2092589	-4.6487185	-3.8290529
H	2.3416102	1.9982580	1.7485529
H	2.0318939	2.0055564	-2.4740591
H	2.4459677	-1.3150908	2.6165816
H	3.8370586	-2.1144902	1.8627256
H	3.9262112	-1.5846905	3.5703277
H	6.0064448	1.0143864	1.8037658
H	6.0381496	-0.2622696	3.0449297
H	5.9640503	-0.7046201	1.3167970
H	4.2461258	0.6913958	4.1803601
H	4.0538179	2.0452874	3.0508477
H	2.6551466	1.0349530	3.4912198
H	1.2843693	4.0804776	-2.2356465
H	-0.0140387	2.8736767	-2.1319909
H	-0.2546011	4.4976307	-1.4592835
H	0.1352380	2.4506917	1.6161411
H	-0.9279638	3.5603281	0.7240695
H	-0.6728540	1.8972705	0.1404048
H	0.9409456	5.2686499	0.5701234
H	2.0298325	4.1849778	1.4610718
H	2.5167808	4.8154038	-0.1224764
H	5.6634414	1.0665893	-3.0292015
H	5.6981151	-0.6607123	-2.5719005
H	5.5397017	-0.1883202	-4.2867783
H	2.0466995	-1.2905555	-3.4134400
H	3.3890930	-1.5104152	-4.5635367
H	3.5371561	-2.0864759	-2.8757304
H	3.6059269	0.7695473	-5.1556372
H	2.1172206	1.0824903	-4.2554765
H	3.5529413	2.1001993	-3.9840119

Vla•⁻.xyz
81
Energy = -1778.210072248

P	2.0585950	-1.2207296	-0.2095828
C	0.2954764	-0.9857897	-0.1521799
C	-0.5384713	-2.1409269	-0.0926198
C	-0.3877270	0.2620016	-0.1660191
C	-1.9135535	-2.0585597	-0.0521462
H	-0.0684833	-3.1246720	-0.0942285
C	-1.7645790	0.3421223	-0.1407278
H	0.1938111	1.1793960	-0.1894999
C	-2.6057654	-0.8088313	-0.0841751
H	-2.4946846	-2.9769145	-0.0311705
H	-2.2296039	1.3246989	-0.1382853
C	-4.0404599	-0.7172915	-0.0665552
C	-4.8466054	-1.7795347	0.5270006
C	-6.1267489	-2.1190423	0.0195674
C	-4.3976045	-2.5263806	1.6455748
C	-6.8958181	-3.1312491	0.5836443
H	-6.5065095	-1.5783701	-0.8430746
C	-5.1661897	-3.5401538	2.2080406
H	-3.4333566	-2.2816221	2.0817626
C	-6.4252966	-3.8578866	1.6844108
H	-7.8676501	-3.3656910	0.1541881
H	-4.7864896	-4.0800229	3.0730138
H	-7.0255481	-4.6496938	2.1242866
C	-4.7172428	0.4405126	-0.6436379
C	-4.2003658	1.1283997	-1.7708257
C	-5.9337692	0.9369029	-0.1097763
C	-4.8464601	2.2323821	-2.3167239
H	-3.2815019	0.7684575	-2.2247289
C	-6.5814436	2.0386616	-0.6586394
H	-6.3600748	0.4467125	0.7611980
C	-6.0457109	2.7031698	-1.7687758
H	-4.4182689	2.7243047	-3.1875386
H	-7.5074507	2.3919896	-0.2096761
H	-6.5507427	3.5650984	-2.1963666
C	2.6314434	0.5553874	-0.2853645
C	2.8543545	1.3024529	0.9151524
C	2.7454763	1.2332115	-1.5359179
C	3.0017617	2.6898335	0.8287479
C	2.8954217	2.6281289	-1.5431403
C	2.9808315	3.3838152	-0.3801188
H	3.1307635	3.2614539	1.7394913
H	2.9371864	3.1421516	-2.4925397
C	2.9818822	0.6687724	2.3258076
C	1.6335587	0.1211249	2.8437421
C	4.0477343	-0.4500368	2.3088910
C	3.4625076	1.6909630	3.3798263
H	0.8772304	0.9136060	2.8461999
H	1.2674441	-0.6967241	2.2217834
H	1.7594801	-0.2417098	3.8722510
H	5.0152956	-0.0467584	1.9879848
H	4.1620630	-0.8655953	3.3180791
H	3.7627424	-1.2596724	1.6313799
H	3.6156958	1.1604089	4.3261168
H	4.4120690	2.1585827	3.0960556
H	2.7237277	2.4797301	3.5607473
C	3.0832866	4.9123096	-0.3846976
C	3.0339574	5.4978797	-1.8051369
C	1.9049261	5.4994896	0.4238598
C	4.4124132	5.3438333	0.2738460
H	3.8728965	5.1452799	-2.4154003
H	2.1014135	5.2325946	-2.3154747
H	3.0918699	6.5908478	-1.7513038
H	1.9149369	5.1377407	1.4569430
H	1.9656351	6.5944620	0.4430099
H	0.9487270	5.2119890	-0.0268278
H	4.4907931	6.4378178	0.2891711
H	4.4794049	4.9825176	1.3050785
H	5.2658467	4.9421989	-0.2835608
C	2.7498134	0.5246039	-2.9169390
C	3.8107313	-0.5989148	-2.9317918
C	1.3615000	-0.0417236	-3.2886287
C	3.1406740	1.4859979	-4.0617005
H	4.8024683	-0.1870629	-2.7113147
H	3.5791955	-1.3721950	-2.1938805
H	3.8407838	-1.0643479	-3.9251601
H	0.6075536	0.7527269	-3.2672462
H	1.3995057	-0.4579715	-4.3039223
H	1.0496712	-0.8247382	-2.5963865
H	3.2152798	0.9036840	-4.9868111
H	2.3890124	2.2665873	-4.2239526
H	4.1099657	1.9651384	-3.8836927

Vla.xyz
81
Energy = -1778.109884427

P	2.0200786	-1.1634965	-0.1686162
C	0.2986579	-0.9471975	-0.1324979
C	-0.5212120	-2.1285961	-0.0595540
C	-0.3975424	0.3088444	-0.1668066
C	-1.8825928	-2.0632239	-0.0158557
H	-0.0301849	-3.0997681	-0.0563612
C	-1.7593343	0.3736259	-0.1563087
H	0.1852585	1.2242690	-0.1861732
C	-2.5862333	-0.8051882	-0.0751136
H	-2.4599580	-2.9816921	0.0077955
H	-2.2446749	1.3443847	-0.1526131
C	-3.9837426	-0.7284386	-0.0524684
C	-4.8119287	-1.8533942	0.4096702
C	-6.0124157	-2.1780372	-0.2534789
C	-4.4545589	-2.6107713	1.5428604
C	-6.8058252	-3.2362076	0.1799747
H	-6.3079577	-1.6002606	-1.1243436
C	-5.2545862	-3.6621383	1.9822888
H	-3.5567727	-2.3460976	2.0934122
C	-6.4302051	-3.9846614	1.2992163
H	-7.7191964	-3.4792696	-0.3558605
H	-4.9663237	-4.2244299	2.8661046
H	-7.0525017	-4.8068900	1.6407349
C	-4.6959777	0.4816765	-0.4917322
C	-4.2912914	1.1969972	-1.6364401
C	-5.8315845	0.9373735	0.2075357
C	-4.9796356	2.3340722	-2.0505836
H	-3.4478905	0.8321557	-2.2152779
C	-6.5133817	2.0794158	-0.2018516
H	-6.1634238	0.3941603	1.0874883
C	-6.0895893	2.7849878	-1.3317565
H	-4.6574405	2.8636112	-2.9429035
H	-7.3772801	2.4217176	0.3611475
H	-6.6250304	3.6735136	-1.6538718
C	2.6103335	0.5882797	-0.2725733
C	2.8282191	1.3461920	0.9195555
C	2.7452628	1.2264966	-1.5393095
C	2.9963301	2.7278564	0.8034899
C	2.9161289	2.6175851	-1.5714013
C	2.9997602	3.3949749	-0.4216801
H	3.1264892	3.3154831	1.7034620
H	2.9801368	3.1095785	-2.5311139
C	2.9297439	0.7282382	2.3379596
C	1.5586652	0.2534515	2.8702623
C	3.9349208	-0.4443811	2.3396106
C	3.4652221	1.7473562	3.3676265
H	0.8261331	1.0663532	2.8259992
H	1.1673753	-0.5894715	2.2987319
H	1.6652085	-0.0599523	3.9158228
H	4.9187440	-0.1069354	1.9958774
H	4.0364973	-0.8404901	3.3567962
H	3.6089566	-1.2665875	1.6934746
H	3.6105225	1.2286695	4.3210899
H	4.4277796	2.1706927	3.0609054
H	2.7608971	2.5674647	3.5435678
C	3.1263439	4.9206606	-0.4573502
C	3.0947570	5.4766636	-1.8900253
C	1.9525110	5.5413862	0.3329143
C	4.4591851	5.3418089	0.2009747
H	3.9337943	5.1021272	-2.4868378
H	2.1620739	5.2148454	-2.4020787
H	3.1669692	6.5691772	-1.8573931
H	1.9503597	5.2017566	1.3735121
H	2.0325959	6.6347338	0.3299669
H	0.9938441	5.2624878	-0.1180232
H	4.5550632	6.4339227	0.1916942
H	4.5136938	5.0041394	1.2408645
H	5.3091564	4.9141364	-0.3418176
C	2.7545035	0.4778122	-2.8973783
C	3.7495883	-0.7026281	-2.8528742
C	1.3497071	-0.0268510	-3.2978836
C	3.2327976	1.3897486	-4.0490433
H	4.7547383	-0.3479547	-2.5999881
H	3.4581487	-1.4604200	-2.1174499
H	3.7865814	-1.1885360	-3.8349462
H	0.6280983	0.7970513	-3.2876921
H	1.3893507	-0.4401031	-4.3130161
H	0.9875639	-0.8053104	-2.6250965
H	3.3212481	0.7809212	-4.9550170
H	2.5224104	2.1953336	-4.2633055
H	4.2125052	1.8325085	-3.8396353

Vla•⁺.xyz
81
Energy = -1777.932430211

P	2.0455271	-1.1115047	0.0593893
C	0.2802685	-0.9207381	-0.0161667
C	-0.4954230	-2.1117324	-0.0526471
C	-0.4000477	0.3260092	0.0140104
C	-1.8712320	-2.0608180	-0.0833025
H	0.0089991	-3.0737542	-0.0831933
C	-1.7729158	0.3781366	-0.0300931
H	0.1767030	1.2424393	0.0808524
C	-2.5547641	-0.8122107	-0.0880372
H	-2.4435685	-2.9785204	-0.1635821
H	-2.2794410	1.3354772	0.0313234
C	-3.9851780	-0.7483989	-0.1523048
C	-4.7977905	-1.8262607	0.3806307
C	-6.0241985	-2.1717538	-0.2344905
C	-4.3904325	-2.5423238	1.5309512
C	-6.7998982	-3.2051855	0.2723351
H	-6.3314939	-1.6506399	-1.1352006
C	-5.1825932	-3.5593307	2.0450413
H	-3.4747973	-2.2569329	2.0386541
C	-6.3844615	-3.8985284	1.4141021
H	-7.7268293	-3.4773603	-0.2224466
H	-4.8724507	-4.0839005	2.9432058
H	-6.9980152	-4.7001751	1.8138725
C	-4.6359270	0.4001838	-0.7578328
C	-4.0566198	1.0592200	-1.8677733
C	-5.8701509	0.8748789	-0.2559290
C	-4.6891459	2.1490614	-2.4496562
H	-3.1371625	0.6711029	-2.2946431
C	-6.4857513	1.9793811	-0.8292820
H	-6.3100735	0.3944714	0.6117898
C	-5.9001547	2.6169596	-1.9280644
H	-4.2495076	2.6304679	-3.3175541
H	-7.4198633	2.3501130	-0.4193940
H	-6.3883175	3.4750578	-2.3798904
C	2.5989626	0.6169860	-0.1493126
C	2.9775377	1.3614395	1.0121958
C	2.5434117	1.2605355	-1.4170476
C	3.1321860	2.7402470	0.8847946
C	2.7088096	2.6506812	-1.4586419
C	2.9622660	3.4174898	-0.3264724
H	3.3932635	3.3174621	1.7626961
H	2.6430656	3.1459261	-2.4178681
C	3.2488482	0.7028470	2.3820014
C	1.9799713	0.0453983	2.9615614
C	4.3661407	-0.3533457	2.2298624
C	3.7349171	1.7246857	3.4292672
H	1.1423041	0.7494844	2.9893220
H	1.6672271	-0.8298697	2.3737061
H	2.1775660	-0.3131249	3.9777361
H	5.2839765	0.1109347	1.8555524
H	4.5765295	-0.8138462	3.2013478
H	4.0838358	-1.1561738	1.5389342
H	3.9545833	1.1905263	4.3589578
H	4.6509962	2.2309448	3.1081958
H	2.9728505	2.4796890	3.6496843
C	3.0975462	4.9407247	-0.3701199

C	2.8746098	5.5061922	-1.7816111
C	2.0488647	5.5624648	0.5798795
C	4.5130793	5.3418197	0.1027492
H	3.6199163	5.1290940	-2.4905782
H	1.8769704	5.2593148	-2.1619265
H	2.9623000	6.5971531	-1.7523674
H	2.1872425	5.2156422	1.6088047
H	2.1399086	6.6543058	0.5726592
H	1.0339639	5.2978348	0.2633123
H	4.6161631	6.4325155	0.0845512
H	4.7055791	4.9996188	1.1244920
H	5.2768869	4.9102350	-0.5528370
C	2.3508716	0.5374178	-2.7707432
C	2.9252632	-0.8849841	-2.7564054
C	0.8576940	0.4862384	-3.1671405
C	3.1085734	1.2850176	-3.8959243
H	3.9843390	-0.8935636	-2.4813216
H	2.3919255	-1.5451758	-2.0449191
H	2.8038454	-1.3528468	-3.7393389
H	0.4180595	1.4886692	-3.1399689
H	0.7621337	0.0943379	-4.1859809
H	0.2834745	-0.1600111	-2.4996590
H	3.0943350	0.6670750	-4.7995398
H	2.6375331	2.2390849	-4.1493194
H	4.1510177	1.4713359	-3.6189056

TS24n.xyz
103
Energy = -3195.556207603

P	0.9765725	-0.1334244	-0.7591819
C	-0.4830855	-1.1113507	-0.2456541
W	2.9928679	-0.1410093	0.8777393
C	0.4660427	1.6436711	-1.5299372
Cl	1.3539143	-1.1701966	-2.5620730
C	-0.9098412	-0.8221987	1.1336746
C	-1.6034488	-1.1609952	-1.1954544
C	4.0265361	-1.2346247	-0.5279211
C	3.8251074	1.6327651	0.2146501
C	4.6261872	-0.2733488	2.0506393
C	2.0966891	0.9041619	2.4134130
C	2.3220090	-1.7770855	1.9029148
C	0.5559657	2.6069817	-0.3405963
C	1.4455396	2.0783613	-2.6325274
C	-0.9491688	1.5772948	-2.1252224
H	-0.0829845	-2.5278775	-0.2521205
C	-2.1996729	-0.5657456	1.4651818
H	-0.1503904	-0.8196991	1.9116100
C	-2.8973670	-0.9809208	-0.8399207
H	-1.3679654	-1.3903371	-2.2282733
O	4.6641844	-1.8367255	-1.2784823
O	4.3872257	2.6083129	-0.0431750
O	5.5741952	-0.3666757	2.7124899
O	1.6873863	1.4131405	3.3666260
O	2.0078780	-2.6246524	2.6286269
C	-0.2151494	2.3843052	0.8119690
C	1.3362820	3.7689018	-0.3903449
C	1.0284862	3.0875319	-3.5165252
C	2.7557533	1.6101608	-2.7539072
C	-2.0662808	2.1751706	-1.5300437
C	-1.1325097	0.9413738	-3.3654130
N	-0.0921079	-3.8911865	-0.2287516
C	-3.2793164	-0.5546273	0.4918480
H	-2.4510663	-0.3957683	2.5079497
H	-3.6625548	-1.0589652	-1.6031175
C	-0.2150806	3.2912197	1.8681590
H	-0.8204978	1.4876619	0.8894121
C	1.3495733	4.6713090	0.6746218
H	1.9557432	3.9670463	-1.2559780
C	1.8895661	3.6048753	-4.4815743
H	0.0190515	3.4794784	-3.4389976
C	3.6235886	2.1209922	-3.7193864
H	3.1187252	0.8371293	-2.0871880
C	-3.3314366	2.0783414	-2.1096367
H	-1.9641785	2.7281558	-0.6051343
C	-2.3926501	0.8442158	-3.9471819
H	-0.2772630	0.5144757	-3.8744570
C	-0.8562864	-4.2418829	1.0208171
C	1.2765318	-4.4938998	-0.0936448
C	-0.7779075	-4.3202218	-1.4839587
C	-4.5599848	-0.1211625	0.8022945
C	0.5601228	4.4484210	1.8015790
H	-0.8202261	3.0871719	2.7478398
H	1.9681901	5.5617970	0.6083603
C	3.1960031	3.1225270	-4.5882155
H	1.5372272	4.3877627	-5.1467769
H	4.6347522	1.7303956	-3.7894704
C	-3.5064834	1.3996644	-3.3130569
H	-4.1793539	2.5374301	-1.6109093
H	-2.5065452	0.3346261	-4.9003661
C	-2.3648944	-4.0553423	0.9381823
H	-0.4378738	-3.6097535	1.8095332
H	-0.6233283	-5.2822391	1.2766871
C	2.1753198	-4.3772780	-1.3140947
H	1.1379120	-5.5508401	0.1649034
H	1.7361873	-4.0171917	0.7717808
C	-0.9386959	-5.8320626	-1.6364503
H	-0.1997107	-3.9042258	-2.3121578
H	-1.7487313	-3.8226386	-1.4932296
C	-4.8318632	0.6567561	2.0267065
C	-5.6987513	-0.3263532	-0.1130172
H	0.5594395	5.1581007	2.6239119
H	3.8668053	3.5226238	-5.3432616
H	-4.4921572	1.3183773	-3.7603027
H	-2.7783745	-4.1791999	1.9432362
H	-2.6316627	-3.0577769	0.5848623
H	-2.8344328	-4.7986099	0.2875972
H	3.1537933	-4.7886355	-1.0528261
H	1.7911539	-4.9436870	-2.1665999
H	2.3108375	-3.3407591	-1.6215402
H	-1.4835966	-6.0362494	-2.5627064
H	0.0263024	-6.3415595	-1.6991494
H	-1.5044724	-6.2668994	-0.8073234
C	-5.9934215	0.4296888	2.7896700
C	-3.9761741	1.6987658	2.4329819
C	-5.9412466	-1.5676974	-0.7333018
C	-6.5960500	0.7243474	-0.3806790
C	-6.2626002	1.1802326	3.9316676
H	-6.6802167	-0.3547273	2.4830330
C	-4.2476589	2.4567579	3.5693022
H	-3.1034189	1.9220836	1.8268329
C	-7.0181139	-1.7428363	-1.5992052
H	-5.2877938	-2.4055397	-0.5047591
C	-7.6674607	0.5546665	-1.2542213
H	-6.4354848	1.6870981	0.0964526
C	-5.3896015	2.1973475	4.3314880
H	-7.1599692	0.9745748	4.5096169
H	-3.5733009	3.2602062	3.8540068
C	-7.8813652	-0.6788373	-1.8747621
H	-7.1880618	-2.7134662	-2.0571126
H	-8.3352275	1.3884150	-1.4563864
H	-5.6045340	2.7868850	5.2176792
H	-8.7213716	-0.8151512	-2.5511766

TS24.xyz
81
Energy = -2902.906575416

P	-0.8417549	0.4701318	0.0599192
Cl	-0.7476055	1.0523814	3.2485701
C	0.8103723	0.2322448	0.7427403
W	-2.5737575	-1.2656036	0.2883857
C	-1.0263008	2.0995683	-0.8863436
H	0.2139058	0.4527472	1.8566536
C	1.2972220	-1.1556359	0.6789277
C	1.8774645	1.2399594	0.7200025
C	-3.6206584	-0.2763433	1.7828815
C	-3.8630569	-0.4030960	-1.0691977
C	-3.8987666	-2.8058874	0.4131283
C	-1.5580106	-2.3174702	-1.1782762
C	-1.5370307	-2.1805123	1.8247131
C	-0.5794086	1.3398346	-2.1456428
C	-2.4765897	2.5713860	-0.8656820
C	-0.1714276	3.3001201	-0.4952009
C	2.6102960	-1.4638746	0.5847086
H	0.5697168	-1.9578063	0.6962543
C	3.1906860	0.9041192	0.6792706
H	1.6042429	2.2833778	0.7806724
O	-4.2339379	0.2237571	2.6168261
O	-4.6674690	0.0206924	-1.7799262
O	-4.6379285	-3.6924574	0.4715738
O	-1.0004222	-2.9170994	-1.9889650
O	-1.0493442	-2.7212116	2.7176947
C	0.7976359	1.1034187	-2.3689334
C	-1.5058170	0.7726750	-3.0438391
C	-3.0327529	3.2013084	-1.9857059
C	-3.2160115	2.5194892	0.3198552
C	0.5568542	4.0089680	-1.4544587
C	-0.2156136	3.7787576	0.8209296
C	3.6532209	-0.4597474	0.5728266
H	2.8974989	-2.5095381	0.5542411
H	3.9254449	1.7025533	0.6701040
C	1.2228550	0.3422145	-3.4498765
H	1.5289620	1.5180761	-1.6843967
C	-1.0724093	0.0178893	-4.1281141
H	-2.5646817	0.9331972	-2.8944224
C	-4.3274126	3.7152884	-1.9331886
H	-2.4537974	3.2965384	-2.8993212
C	-4.5098614	3.0351421	0.3748365
H	-2.7637672	2.0915590	1.2108962
C	1.2614861	5.1601300	-1.0950825
H	0.5767452	3.6702187	-2.4853718
C	0.4934505	4.9211765	1.1792087
H	-0.7659564	3.2265630	1.5781453
C	5.0021901	-0.7815161	0.4588142
C	0.2905294	-0.2021551	-4.3368886
H	2.2850519	0.1761503	-3.6015548
H	-1.8034556	-0.4039625	-4.8105884
C	-5.0748060	3.6236338	-0.7568303
H	-4.7504292	4.1914575	-2.8129070
H	-5.0726224	2.9765932	1.3017140
C	1.2387057	5.6162000	0.2223364
H	1.8278514	5.6972932	-1.8503180
H	0.4701805	5.2644869	2.2093083
C	5.4451827	-2.1071923	-0.0081219
C	6.0617568	0.1874745	0.7912481
H	0.6233419	-0.7950569	-5.1831654
H	-6.0855667	4.0189714	-0.7204745
H	1.7945206	6.5061008	0.5025805
C	6.5432856	-2.7480587	0.5966146
C	4.8187660	-2.7469892	-1.0947642
C	5.9840716	0.9903387	1.9451791
C	7.2053555	0.3022561	-0.0218667
C	6.9763825	-3.9938233	0.1529487
H	7.0443181	-2.2622248	1.4287365
C	5.2597394	-3.9882338	-1.5441938
H	3.9986295	-2.2460115	-1.6009615
C	6.9990651	1.8892860	2.2600240
H	5.1302822	0.8805639	2.6074167
C	8.2144021	1.2082318	0.2888732
H	7.2858001	-0.3190310	-0.9090534
C	6.3361024	-4.6203504	-0.9184289
H	7.8154436	-4.4785122	0.6441255
H	4.7698833	-4.4586331	-2.3921324
C	8.1154746	2.0072345	1.4301353
H	6.9243242	2.4909838	3.1614781
H	9.0808714	1.2929841	-0.3609951
H	6.6791602	-5.5894545	-1.2689159
H	8.9070726	2.7090882	1.6760185

TS34n.xyz
103
Energy = -3195.577486250

P	1.5143299	0.5015873	-0.4286832
Cl	1.5994596	1.0900795	-2.4497483
C	-0.2672928	0.4773127	-0.2083595
W	2.7015727	-1.7613466	-0.1532037
C	2.1434885	2.0841782	0.5327819
C	-0.8674053	-0.5437976	0.5538068
C	-1.1183950	1.4604659	-0.7540677
C	3.5869820	-1.5311553	-1.9974189
C	4.4325389	-1.0650702	0.7291236
C	3.4834749	-3.6155436	-0.0688402
C	1.9402611	-2.1065869	1.7325404
C	1.0367609	-2.5480920	-1.0760101
C	2.1480913	1.5458728	1.9752648
C	3.5535141	2.5140868	0.1050134
C	1.1969602	3.2641541	0.2725055
C	-2.2314632	-0.5792848	0.7694788
H	-0.2468354	-1.3163812	0.9933609
C	-2.4833093	1.4177782	-0.5468243
H	-0.7043839	2.2576565	-1.3608690
O	4.1164392	-1.4443401	-3.0211383
O	5.4444314	-0.7698420	1.2016632
O	3.9172358	-4.6924866	-0.0275136
O	1.5644360	-2.3875524	2.7882359
O	0.1271363	-3.0227100	-1.6096447
C	0.9601590	1.1664728	2.6279896
C	3.3558837	1.3502962	2.6619810
C	4.0478367	3.7088626	0.6550229
C	4.3746662	1.8027611	-0.7686135
C	0.2535690	3.7362780	1.1922890
C	1.2979227	3.9309144	-0.9617433
C	-3.1101824	0.3931502	0.2150303
H	-2.6413340	-1.3982399	1.3509454
H	-3.0975394	2.1855058	-1.0047232
C	0.9805699	0.6477017	3.9212030
H	0.0087502	1.2648973	2.1239753
C	3.3771628	0.8253903	3.9537294
H	4.2927871	1.6121212	2.1863381
C	5.3255895	4.1656055	0.3483839
H	3.4193558	4.2807662	1.3317847
C	5.6573673	2.2589241	-1.0851040
H	4.0241123	0.8819327	-1.2176856
C	-0.6042271	4.7888833	0.8672658
H	0.1836938	3.3000251	2.1797426

C	0.4372873	4.9735619	-1.2921489
H	2.0624236	3.6293162	-1.6674184
C	-4.5601775	0.2325050	0.2369442
C	2.1889973	0.4770205	4.5946268
H	0.0446734	0.3671276	4.3957262
H	4.3303780	0.6877360	4.4560287
C	6.1394095	3.4399892	-0.5274982
H	5.6863662	5.0900372	0.7906320
H	6.2738151	1.6847266	-1.7709577
C	-0.5333519	5.3996419	-0.3824882
H	-1.3297237	5.1276016	1.6015415
H	0.5305956	5.4580344	-2.2601099
C	-5.2158230	-0.4571555	1.3978895
C	-5.3721492	1.4378646	-0.1830506
H	-4.5340376	-0.8642463	-0.8720247
H	2.2053960	0.0676944	5.6004393
H	7.1359230	3.7962761	-0.7723000
H	-1.2085442	6.2111080	-0.6384816
C	-6.5107273	-0.9938737	1.2535407
C	-4.6247802	-0.5571302	2.6710156
C	-6.4114085	1.3691641	-1.1205068
C	-5.1386090	2.6828488	0.4299341
N	-4.3490120	-1.7591907	-1.7636752
C	-7.1647746	-1.6268740	2.3070844
H	-7.0119493	-0.9102790	0.2930888
C	-5.2717370	-1.1985086	3.7278029
H	-3.6491574	-0.1118818	2.8410844
C	-7.1820614	2.4892144	-1.4428856
H	-6.6297171	0.4232917	-1.6056859
C	-5.8943998	3.8075648	0.1078747
H	-4.3455049	2.7616019	1.1694545
C	-3.6961764	-2.9602925	-1.1407514
C	-3.3694585	-1.1568204	-2.7311298
C	-5.6738458	-2.0793011	-2.3810987
C	-6.5439157	-1.7464404	3.5534486
H	-8.1605183	-2.0350935	2.1528679
H	-4.7826995	-1.2576371	4.6972461
C	-6.9236282	3.7164321	-0.8338340
H	-7.9809543	2.4004566	-2.1746503
H	-5.6876599	4.7557641	0.5979198
C	-4.5328350	-3.6520279	-0.0749115
H	-2.7595167	-2.5937628	-0.7180412
H	-3.4424411	-3.6574369	-1.9473704
C	-3.8898150	0.0857993	-3.4376076
H	-3.0828223	-1.9291327	-3.4536474
H	-2.4874047	-0.9123454	-2.1346248
C	-5.6371995	-3.1397435	-3.4767014
H	-6.0656977	-1.1414265	-2.7778013
H	-6.3308727	-2.3869599	-1.5649098
H	-7.0466217	-2.2485094	4.3752847
H	-7.5166899	4.5911733	-1.0861245
H	-3.9311370	-4.4516338	0.3680828
H	-4.8284873	-2.9611418	0.7179647
H	-5.4345851	-4.1108435	-0.4910552
H	-3.0625794	0.5433023	-3.9877691
H	-4.6800168	-0.1458085	-4.1579522
H	-4.2685473	0.8198306	-2.7216965
H	-6.6486084	-3.2646565	-3.8746749
H	-4.9849291	-2.8478343	-4.3050885
H	-5.3051713	-4.1101888	-3.0974097

TS4nc.xyz

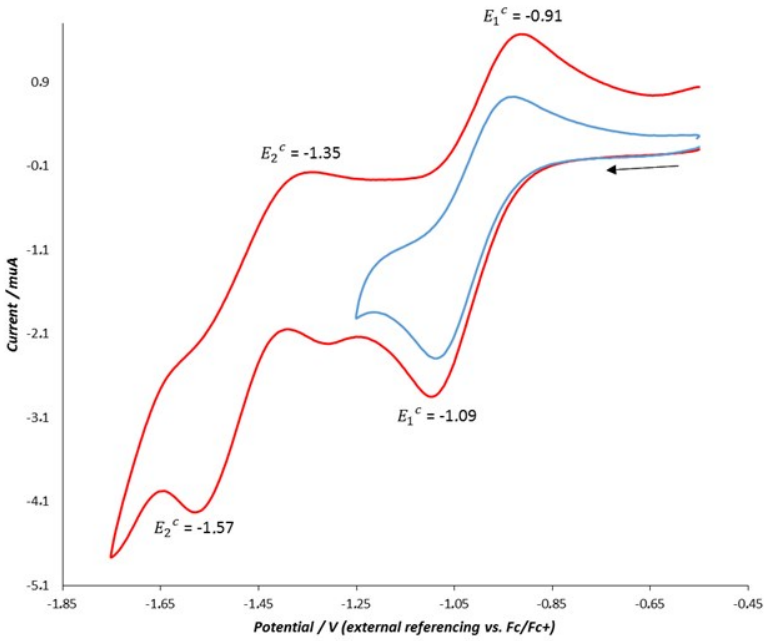
103

Energy = -3195.583610311

C	-7.9134709	1.9720004	0.2066295
C	-6.8471395	2.0459456	-0.6937386
C	-5.8562120	1.0675412	-0.6908073
C	-5.8876084	-0.0140759	0.2133239
C	-6.9824322	-0.0780420	1.1005473
C	-7.9747437	0.8986005	1.1009657
C	-4.8458762	-1.0545495	0.2141523
C	-5.2997082	-2.4471499	0.3203654
C	-6.4984894	-2.8667215	-0.2985438
C	-6.9548744	-4.1775199	-0.1889778
C	-6.2325554	-5.1202433	0.5491845
C	-5.0496681	-4.7240030	1.1816257
C	-4.5940552	-3.4133011	1.0716173
C	-3.4830103	-0.7170100	0.1303687
C	-2.4574160	-1.6614763	-0.2326103
C	-1.1301663	-1.3286371	-0.2742356
C	-0.6539126	-0.0300704	0.0857588
C	-1.6648069	0.9337353	0.3973401
C	-2.9973652	0.6109404	0.4041977
P	1.0641678	0.2839780	0.1203868
Cl	1.2001553	2.1603777	-1.2883622
W	2.6332420	-1.4624399	-0.9069599
C	1.2460188	-1.6069998	-2.4192564
O	0.5253387	-1.6722595	-3.3223340
C	1.4844451	1.1047777	1.8426463
C	0.4280292	2.1305703	2.2729174
C	-0.5180101	1.9055578	3.2781204
C	-1.4759899	2.8723730	3.5918335
C	-1.5013053	4.0891975	2.9145474
C	-0.5242212	4.3499628	1.9493364
C	0.4362656	3.3896840	1.6471308
C	3.5941240	-0.0663017	-2.0732757
O	4.1746893	0.6720624	-2.7488371
C	4.1766870	-1.2998049	0.4518285
O	5.1168587	-1.2571240	1.1231635
C	3.7049712	-2.8977938	-1.8231193
O	4.3046956	-3.7378710	-2.3595405
C	1.7715464	-2.9332571	0.2618387
O	1.3402607	-3.8002345	0.8903824
C	1.5201210	-0.1771335	2.7026605
C	0.3674967	-0.9640527	2.8952039
C	0.4135435	-2.1373376	3.6437017
C	1.6160246	-2.5723355	4.2029113
C	2.7692371	-1.8156887	4.0052259
C	2.7202718	-0.6334152	3.2649328
C	2.8400788	1.8252826	1.8739536
C	3.1944052	2.4648129	3.0742109
C	4.4085145	3.1317664	3.2010533
C	5.2965881	3.1846666	2.1215082
C	4.9507061	2.5645896	0.9240809
C	3.7311772	1.8926114	0.8055752
N	-1.4974820	2.8886513	-2.6784587
C	-2.8245020	3.2148380	-2.0328173
C	-3.8538807	3.7493967	-3.0132741
C	-1.5672207	1.7896501	-3.7244815
C	-2.2981240	0.5485885	-3.2446845
C	-0.7870359	4.0944747	-3.2629682
C	-0.5910364	5.2135612	-2.2528926
H	-0.8585093	2.5303883	-1.9361600
H	-0.4140835	-2.0884549	-0.5651366
H	-1.3786736	1.9497550	0.6424609
H	-2.7484871	-2.6687164	-0.5114668
H	-3.7140170	1.3784139	0.6810029
H	-0.5703246	-0.6689672	2.4422708
H	3.6298307	-0.0634243	3.1243562
H	2.5065990	2.4347376	3.9147837
H	3.4772643	1.4249386	-0.1353100
H	-0.5202089	0.9731892	3.8281858
H	1.2018378	3.6050577	0.9117485
H	-0.4936250	-2.7201808	3.7744725
H	3.7172401	-2.1431270	4.4225864
H	4.6617135	3.6135336	4.1415789
H	5.6243211	2.6017074	0.0723250
H	-2.2057166	2.6646618	4.3692799
H	-0.5036152	5.3099599	1.4402649
H	-0.5238840	1.5659061	-3.9587367
H	-2.0337515	2.2287567	-4.6083298
H	-1.3685206	4.4158215	-4.1288630
H	0.1739065	3.7122789	-3.6134191
H	-2.6081043	3.9370268	-1.2435558
H	-3.1520951	2.2931832	-1.5517120
H	1.6536394	-3.4939370	4.7765556
H	6.2441248	3.7077558	2.2164297
H	-2.2544179	4.8353757	3.1510170
H	-2.1637446	-0.2338160	-3.9960665
H	-1.8940425	0.1801439	-2.2986608
H	-3.3718341	0.7186455	-3.1300774
H	0.0528881	5.9725983	-2.7051862
H	-1.5323063	5.6958736	-1.9776334
H	-0.0960497	4.8431108	-1.3502514
H	-3.5312459	4.6810359	-3.4858796
H	-4.7731911	3.9610434	-2.4611630
H	-4.0920078	3.0220959	-3.7941753
H	-7.0701667	-2.1462374	-0.8770140
H	-3.6891377	-3.1144057	1.5931543
H	-5.0504541	1.1092268	-1.4184871
H	-7.0398333	-0.9062684	1.8013869
H	-7.8770213	-4.4679101	-0.6867616
H	-4.4872713	-5.4393542	1.7769244
H	-6.8033770	2.8589863	-1.4143194
H	-8.7993637	0.8261651	1.8058671
H	-6.5879107	-6.1431629	0.6362845
H	-8.6895935	2.7322397	0.2042474

Results and Discussion

Cyclic voltammograms of **4** were obtained at room temperature in both CH_3CN and THF solution containing 2 mM of **4** and 0.1 M $^nBu_4NBF_4$ as the supporting electrolyte. The used CH_3CN was bought from Wako (H_2O < 0.001 %) and the THF was pre-dried via distillation over sodium wire then dried over potassium before re-condensation. The measurements were done under inert atmosphere in the glovebox. The measurements were performed with a Pine Research WaveNow potentiostat over scan rates of 20 mV s^{-1} – 1500 mV s^{-1}. Ceramic Patterned Electrodes (CPE) with working surfaces of Pt or Au were used in a glass vial cell with a special PTFE insert at the bottom for small volumes. Potentials are quoted versus the operative formal potential E^{0}_{Fc/Fc^+} for the Cp_2Fe redox couple – abbreviated as Fc/Fc^+ - which was used as an external standard for **4**, measured in the same solvent (E^{0}_{Fc/Fc^+}(CH_3CN): 0,440 V,



E^{0}_{Fc/Fc^+} (THF): 0,550 V).

Figure S3. Cyclic voltammograms on solutions of **4** in THF (2 mM of **4**, 0.2 M $^nBu_4NPF_6$, 50 mV/s red, 100 mV/s blue).

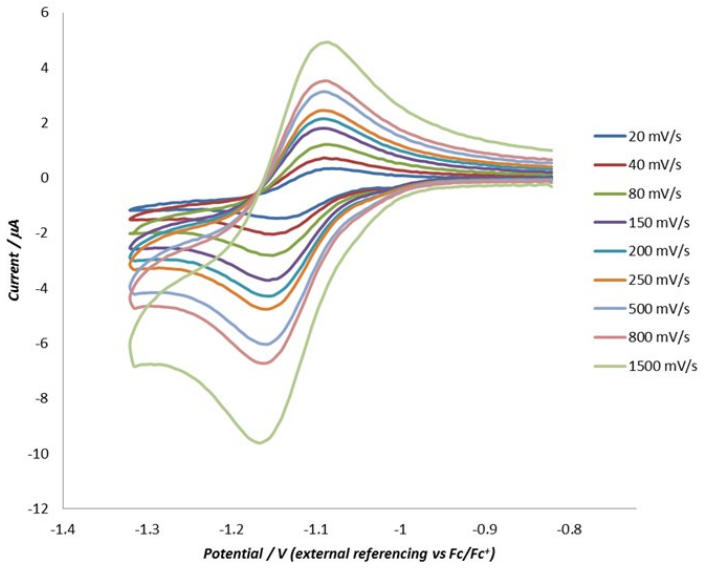


Figure S4. Cyclic voltammograms on solutions of **4** in MeCN (2 mM of **4**, 0.1 M $^{n}Bu_4NPF_6$).

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