Supplementary information for:

An untethered C_{3v}-symmetric triarylphosphine oxide locked by intermolecular hydrogen bonding

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1. Materials and Physical Measurements

General Considerations. All manipulations were performed under an atmosphere of dry, oxygen-free N_2 by means of standard Schlenk or glovebox techniques (MBraun UNIlab Pro SP Eco equipped with a -38 °C freezer). Pentane, toluene, benzene, ether, tetrahydrofuran (THF), and dichloromethane (DCM) were dried using an MBraun solvent purification system. All solvents were degassed by freeze-pump-thaw and stored on activated 4 Å molecular sieves prior to use. Trimethylsilyl chloride and triethylamine were purchased from Aldrich and freshly distilled before use. AgF was purchased from Aldrich and $[Ph_3C][B(C_6F_5)_4]$ was purchased from Strem Chemicals and both were used without further purification. Cp_2VF,[1] $P(O)(C_6H_4$-*p*-$COOH)_3$,[2] and $Ph_2P(O)(C_6H_4$-p-$COOH)$[3] were prepared according to literature procedures. Elemental analyses (C, N, H) were recorded at the University of California, Berkeley using a Perkin Elmer 2400 Series II combustion analyzer.

Spectroscopic Analysis: NMR spectra were obtained on an Agilent Technologies 400 MHz spectrometer, and referenced to residual solvent or externally (^{11}B: $BF_3{\cdot}Et_2O$; ^{19}F: $CFCl_3$; ^{31}P: 85% H_3PO_4). Chemical shifts (δ) are recorded in ppm and the coupling constants are in Hz. X-band EPR spectra were collected on a Bruker EMX EPR Spectrometer equipped with an Oxford ESR 900 liquid helium cryostat. A modulation frequency of 100 kHz was used for all EPR spectra. UV-Vis spectroscopy was performed using a Shimadzu UV-2401PC spectrophotometer with quartz cuvettes equipped with air tight J-young adaptors. IR spectra were recorded on a Nicolet 6700 FT-IR spectrometer with a NXR FT Raman Module.

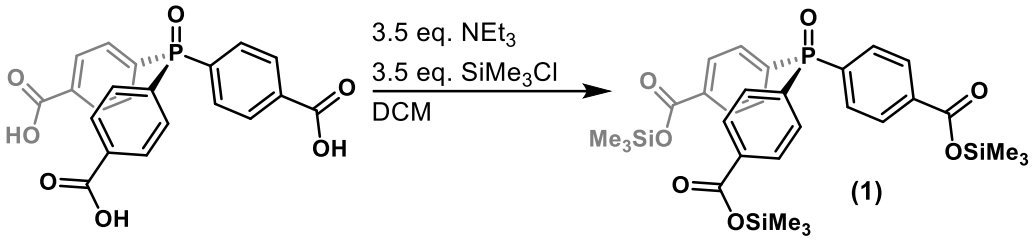
X-ray crystallography: Data was collected on a Bruker KAPPA APEX II diffractometer equipped with an APEX II CCD detector using a TRIUMPH monochromator with a Mo Kα X-ray source (α = 0.71073 Å). The crystals were mounted on a cryoloop with Paratone-N oil, and all data were collected at 100(2) K using an Oxford nitrogen gas cryostream system. A hemisphere of data was collected using ω scans with 0.5° frame widths. Data collection and cell parameter determination were conducted using the SMART program. Integration of the data frames and final cell parameter refinement were performed using SAINT software. Absorption correction of the data was carried out using SADABS. Structure determination was done using direct or Patterson methods and difference Fourier techniques. All hydrogen atom positions were idealized and rode on the atom of attachment. Structure solution, refinement, graphics, and creation of publication materials were performed using SHELXTL.

Electrochemical Analyses: Cyclic voltammetry was performed on a CH Instruments 630E electrochemical analysis potentiostat, equipped with a 3 mm diameter glassy carbon working electrode, a Ag wire pseudo-reference electrode, and a Pt counter electrode with $[Bu_4N][PF_6]$ (0.1 M) supporting electrolyte solution in DCM. The glassy carbon working electrode was cleaned prior to each experiment by polishing with 1, 0.3, 0.05 mm alumina (CH Instruments) in descending order, followed by sonication in distilled water for two minutes. Background scans were conducted for each experiment in a solution containing only electrolyte, and was then subtracted from each experiment. All voltammograms were referenced to the Fc/Fc^+ redox couple.

Electrochemical Simulations: All simulations were performed using DigiSim with the same concentration, starting potential, ending potential, voltage window, and scan rate as experimental data, and the assumption that T = 298.2 K, and $r_{electrode}$ = 1.5 mm. All events were assumed to have an α/ λ ratio of 0.5, and the diffusion coefficient (*Df*) and the heterogeneous charge transfer constant (k_s) were fitted to all scan rates to produce the closest fits. A 1-1.2 kΩ correction factor was found to be necessary to account for the high cell impedance. k_s(**2**) and *Df*(**2**) were found to be 0.007 cm/s and 0.0000045 cm^2/s, respectively. k_s(**4**) and *Df*(**4**) were found to be 0.005 cm/s and 0.000015 cm^2/s respectively.

2. Synthesis of Compounds

2.1 Synthesis of P(O)(C_6H_4-*p*-$COOSiMe_3$)$_3$ (**1**)



A 100 mL Schlenk flask equipped with a stirbar was charged with dry P(O)(C_6H_4-*p*-$COOH)_3$ (0.80 g, 1.95 mmol) and 25 mL of DCM. Using a gas-tight syringe, NEt_3 (0.95 mL, 6.82 mmol) was added dropwise under nitrogen while stirring. The solid dissolved and the solution went clear. After stirring for ten minutes $SiMe_3Cl$ (0.86 mL, 6.82 mmol) was added slowly dropwise using a gas-tight syringe. The resulting solution was allowed to stir for 30 min. and then the volatiles were removed *in vacuo* to afford a white solid. The solid was brought into the glovebox and brought up in benzene (10 mL). The solution was filtered through a fine porosity glass frit over a pad of celite, and then dried *in vacuo* to yield a flaky white solid (0.860 g, 1.37 mmol, 70.5%). ^{1}H NMR (400 MHz, C_6D_6, 25 °C): δ = 8.06-7.97 (m, 6H; *o*-Ar*H*), 7.66-7.56(m, 6H; *m*-Ar*H*), 0.29 (s, 27H; OSi*Me*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2, 25 °C): δ = -0.67 (s, Si(*C*H_3)$_3$), 129.88 (*Ar*), 131.82 (*Ar*), 134.97 (*Ar*), 136.97 (*Ar*), 165.42 (*C*OOSi). $^{31}P\{^1H\}$NMR (162 MHz, C_6D_6, 25 °C): δ = 23.56 (s). MS (APCI) calculated $C_{30}H_{40}O_7PSi_3^+$: 627.178 ($M+H^+$), found: 627.2.

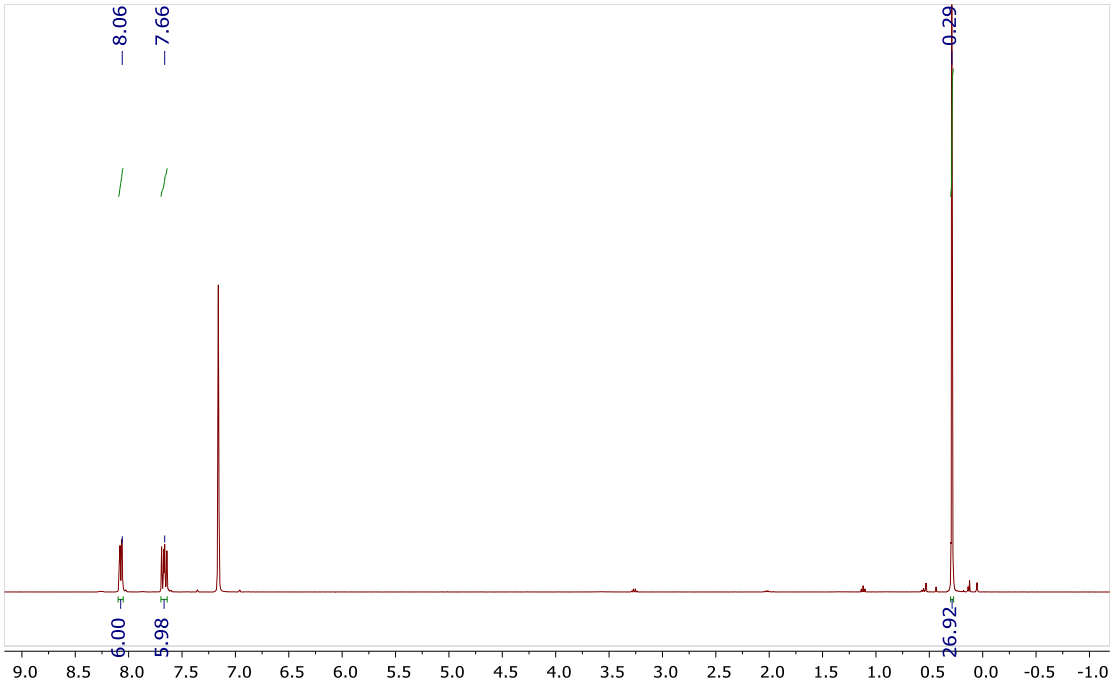


Figure S1: ^{1}H NMR spectrum of P(O)(C_6H_4-*p*-$COOSiMe_3$)$_3$ **(1)** (400 MHz, C_6D_6, 25 ^{o}C).

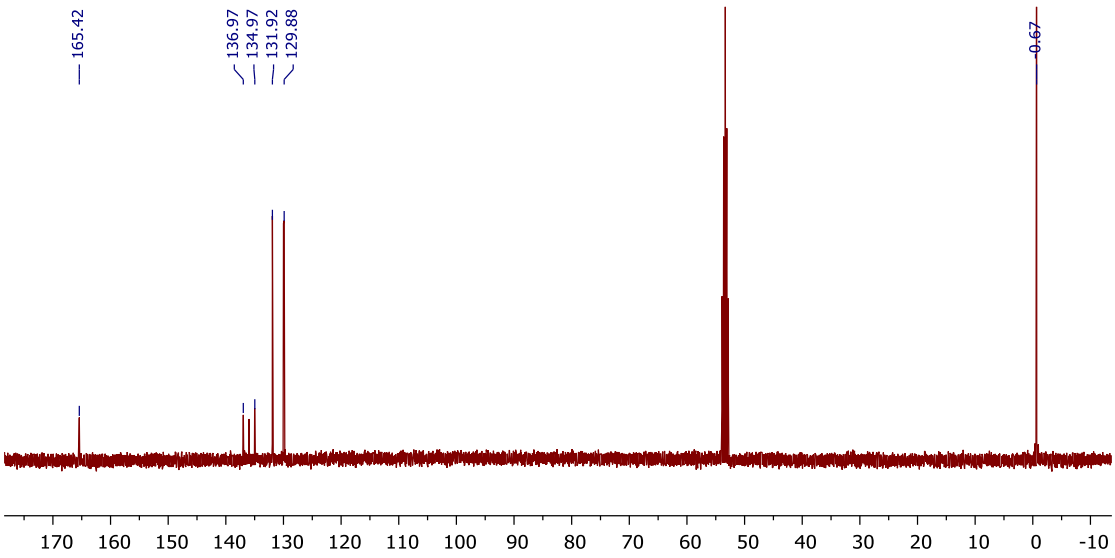


Figure S2: ^{13}C{^{1}H} NMR spectrum of P(O)(C_6H_4-*p*-$COOSiMe_3$)$_3$ (**1**) (100 MHz, CD_2Cl_2, 25 ^{o}C).

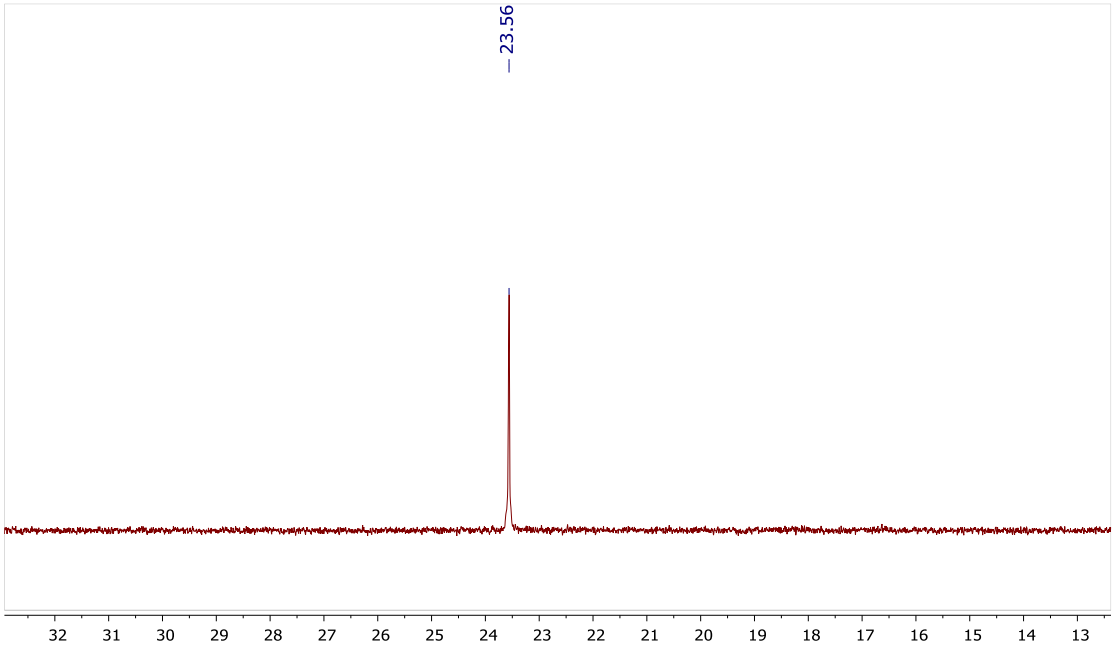
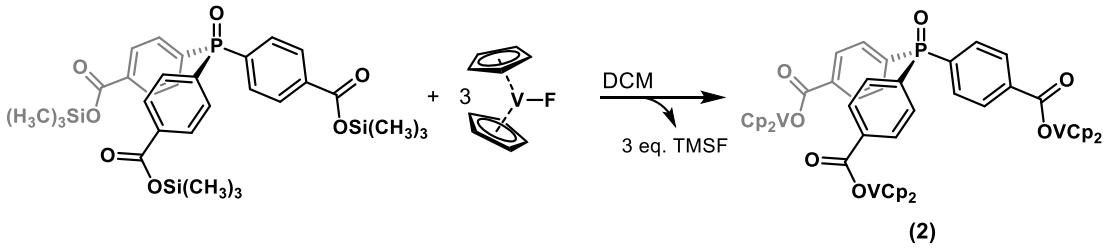


Figure S3: $^{31}P\{^{1}H\}$ NMR spectrum of $P(O)(C_6H_4\text{-}p\text{-}COOSiMe_3)_3$ (**1**) (162 MHz, C_6D_6, 25 °C).

2.2 Synthesis of $P(O)(C_6H_4\text{-}p\text{-}COOVCp_2)_3$ (**2**)



In the glovebox, a solution of $P(O)(C_6H_4\text{-}p\text{-}COOSiMe_3)_3$ (0.21 g, 0.33 mmol) in DCM (3 mL) was added slowly dropwise to a solution of VCp_2F (0.20 g, 1 mmol) in DCM (10 mL). The resulting bright blue solution was allowed to stir at room temperature for 90 min, and then the volatiles were removed *in vacuo* to afford a dark blue residue. The residue was washed with benzene (10 mL) and pentane (2 x 5 mL) and dried *in vacuo* to yield a bright blue solid (0.30 g, 0.32 mmol, 96.9%). Blue plate shaped single crystals suitable for XRD were grown by slow diffusion of pentane into a concentrated solution of **2** in DCM at -40 °C over several days. The product was stored at -40 °C to prevent thermal decomposition. $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2, 25 °C): δ = 26.18 (s). UV-vis: λ (nm): 315.5, 734.5; ε (L mol^{-1} cm^{-1}): 9640, 230. Anal. Calc. for $C_{51}H_{42}O_7PV_3$: C, 64.43; H, 4.45. Found: C, 64.12; H, 4.46.

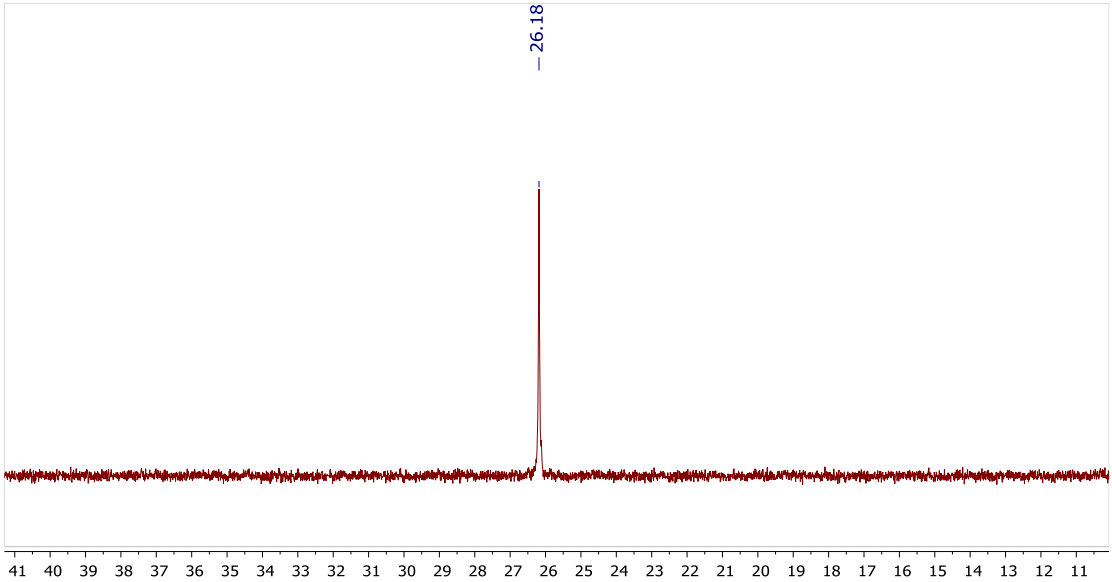
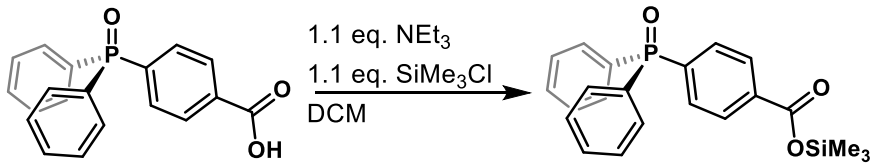


Figure S4: ^{31}P NMR spectrum of $P(O)(C_6H_4$-*p*-$COOVCp_2)_3$ (**2**) (162 MHz, C_6D_6, 25 °C).

2.3 Synthesis of $Ph_2P(O)(C_6H_4$-*p*-$COOSiMe_3)$ (**3**)



A 100 mL Schlenk flask equipped with a stirbar was charged with dry $Ph_2P(O)(C_6H_4$-*p*-COOH) (0.40 g, 1.28 mmol) and 25 mL of DCM. Using a gas-tight syringe, NEt_3 (0.20 mL, 1.42 mmol) was added dropwise under nitrogen while stirring. The solid dissolved and the solution went clear. After stirring for 10 minutes $SiMe_3Cl$ (0.18 mL, 1.42 mmol) was added slowly dropwise at room temperature using a gas-tight syringe. The resulting solution was allowed to stir for 30 mins. and then the volatiles were removed *in vacuo* to afford a white solid. The solid was brought into the glovebox and brought up in benzene (10 mL). The solution was filtered through a fine porosity glass frit over a pad of celite, and then dried *in vacuo* to yield a flaky white solid (0.22 g, 0.55 mmol, 43%). ^1H NMR (400 MHz, C_6D_6, 25 °C): δ = 7.99-8.02 (m, 2H), 7.69-78 (m, 6H), 6.98-7.06 (m, 6H), 0.28 (s, 9H, OSi*Me*$_3$). $^{13}C\{^1H\}$ NMR (100 MHz, CD_2Cl_2, 25 °C): δ = -0.64 (Si(*C*H_3)$_3$), 128.50 (*Ar*), 129.67 (*Ar*), 131.82 (*Ar*), 132.07 (*Ar*), 132.75 (*Ar*), 134.54 (*Ar*), 137.24 (*Ar*), 138.25 (*Ar*), 165.59 (*C*OOSi). $^{31}P\{^1H\}$ (162 MHz, C_6D_6, 25 °C): δ = 23.56 (s). MS (APCI) calculated $C_{22}H_{23}O_3PSi^+$: 395.128 ($M+H^+$), found: 395.1

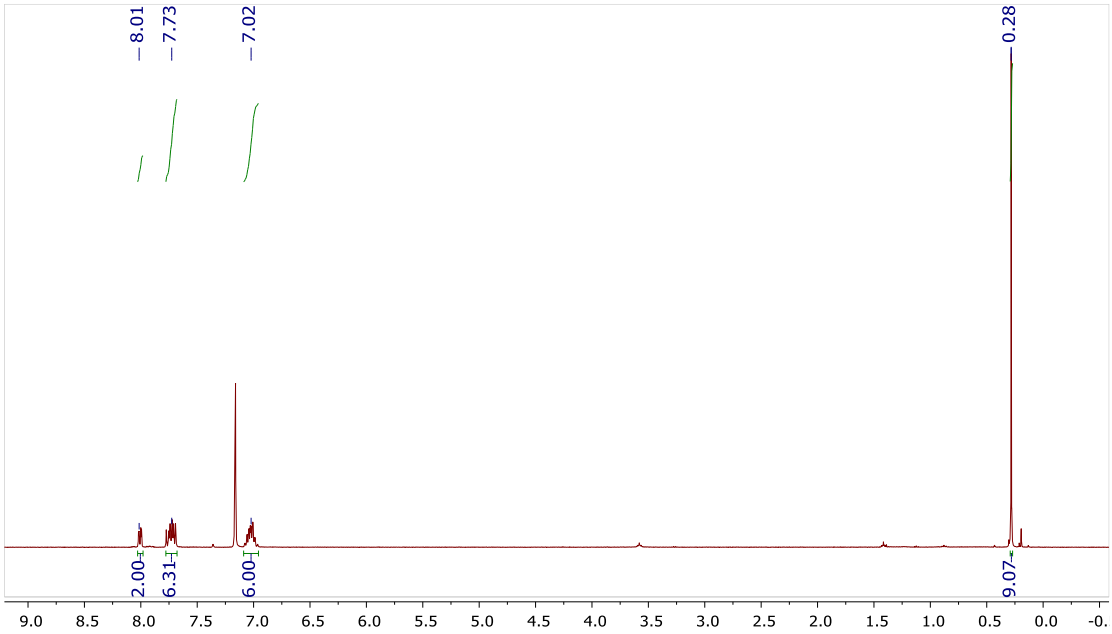


Figure S5: ^{1}H NMR spectrum of $Ph_2P(O)(C_6H_4$-*p*-$COOSiMe_3)_3$ (**3**) (400 MHz, C_6D_6, 25 °C).

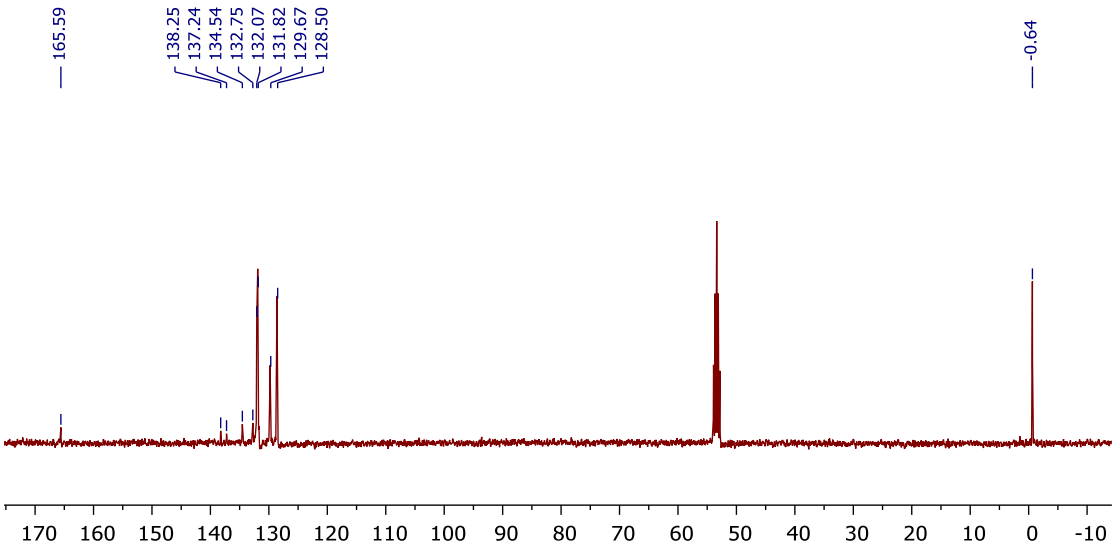


Figure S6: $^{13}C\{^{1}H\}$ NMR spectrum of $Ph_2P(O)(C_6H_4$-*p*-$COOSiMe_3)$ (**3**) (100 MHz, CD_2Cl_2, 25 °C).

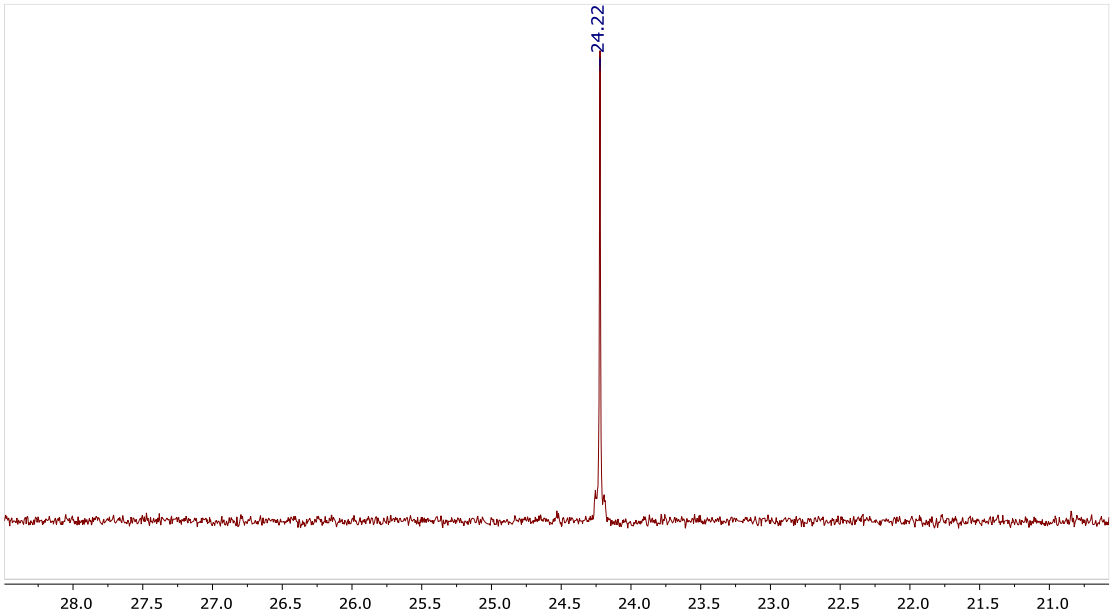
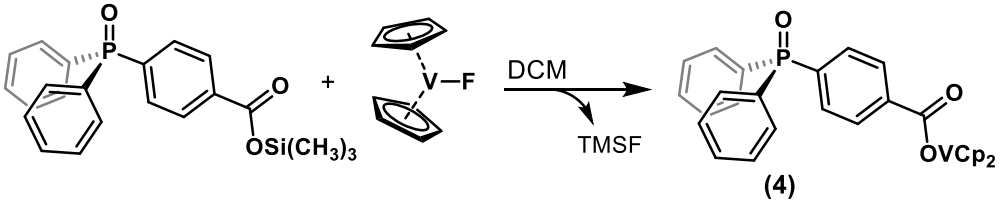


Figure S7: $^{31}P\{^{1}H\}$ NMR spectrum of $Ph_2P(O)(C_6H_4$-*p*-$COOSiMe_3)$ (**3**) (162 MHz, C_6D_6, 25 °C)

2.4 Synthesis of $Ph_2P(O)(C_6H_4$-*p*-$COOVCp_2)$ (**4**)



In the glovebox, a solution of $Ph_2P(O)(C_6H_4$-*p*-$COOSiMe_3)$ (**3**) (0.137 g, 0.346 mmol) in DCM (3 mL) was added slowly dropwise to a solution Cp_2VF (0.069 g, 0.346 mmol) in DCM (10 mL). The resulting bright blue solution was allowed to stir at room temperature for 90 mins, and then the volatiles were removed *in vacuo* to afford a dark blue residue. The residue was washed with diethyl ether (2 x 5 mL) and dried *in vacuo* to yield a bright blue solid (0.141 g, 0.290 mmol, 83.8%). Blue plate-shaped single crystals suitable for XRD studies were grown by slow diffusion of pentane into a concentrated solution of **4** in DCM at -40 °C over three days. The product was stored at -40 °C to prevent thermal decomposition. ^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ = 8.81 (bs, 2H), 7.67 (bm, 4H), 7.57 (bm, 2H), 7.50 (bm, 4H), 6.92 (bs, 2H). ^{31}P NMR (162 MHz, CD_2Cl_2, 25 °C): δ = 26.85 (s). UV-vis: λ (nm): 314, 560, 733; ε ($L\,mol^{-1}\,cm^{-1}$): 3750, 210, 230. μ_{eff}(Evans): 2.74 μ_B. Anal. Calc. for $C_{29}H_{24}O_3PV$: C, 69.33%; H, 4.82%. Found: C, 68.28%; H, 4.67%. Attempts to obtain satisfactory elemental analysis consistently resulted in reduced carbon percentages which we attribute to incomplete combustion as a result of vanadium carbide formation.[4]

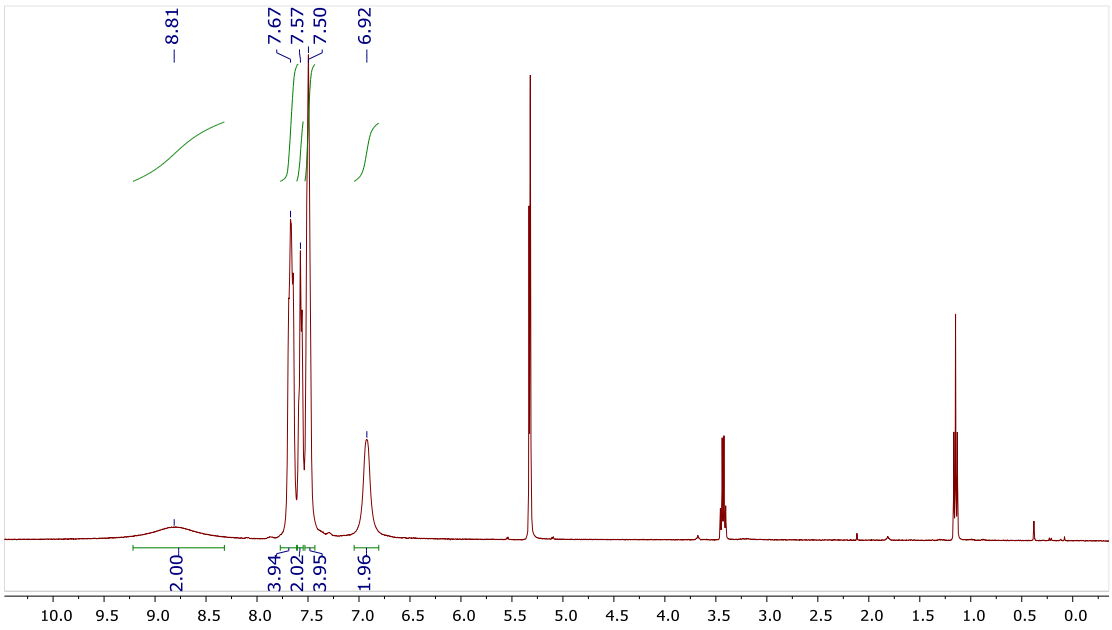


Figure S8: ^{1}H NMR spectrum of $Ph_2P(O)(C_6H_4$-*p*-$COOVCp_2)$ (**4**) (400 MHz, CD_2Cl_2, 25 ºC).

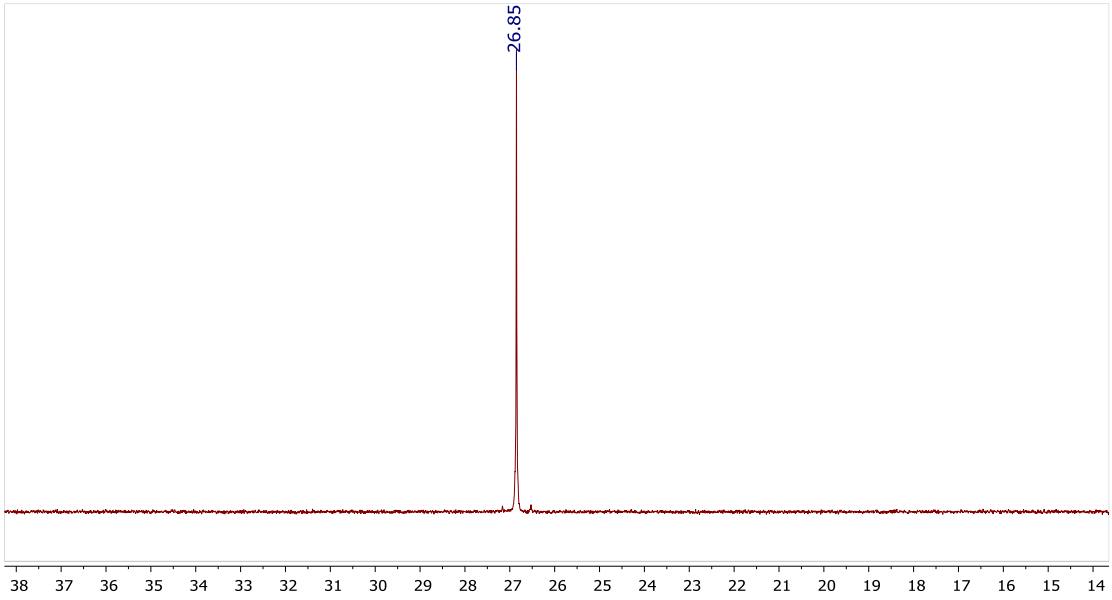
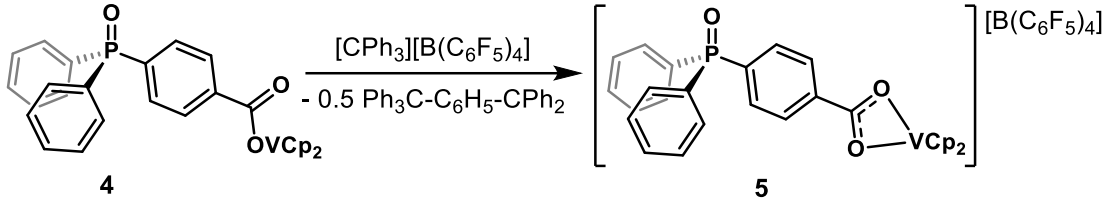


Figure S9: $^{31}P\{^{1}H\}$ NMR spectrum of $Ph_2P(O)(C_6H_4$-*p*-$COOVCp_2)$ (**4**) (162 MHz, C_6D_6, 25 ºC).

2.5 Synthesis of $[Ph_2P(O)(C_6H_4\text{-}p\text{-}COOVCp_2)][B(C_6F_5)_4]$ (**5**)



In the glovebox, a solution $[CPh_3][B(C_6F_5)_4]$ (0.054 g, 0.059 mmol) in DCM (3 mL) was added dropwise to a solution of $Ph_2P(O)(C_6H_4\text{-}p\text{-}COOVCp_2)$ (**4**) (0.030 g, 0.059 mmol) in DCM (3 mL). The solution instantly turned a dark orange and was allowed to stir at room temperature for 30 mins. The volatiles were removed *in vacuo* and the orange/brown residue was washed with benzene (3 x 5 mL). The residue was dissolved in a minimal amount of DCM (1 mL) and carefully layered with hexanes (1 mL). The solution was cooled to -40 °C and left to recrystallize for 24 h. The resulting orange precipitate was filtered and dried *in vacuo*. (0.035 g, 0.030 mmol, 50.8%). Highly air sensitive red plate-shaped single crystals suitable for XRD were grown by slow diffusion of pentane into a concentrated solution of **5** in DCM at -40 °C over several days. The product was stored at -40 °C to prevent thermal decomposition. ^{1}H NMR (400 MHz, CD_2Cl_2, 25 °C): δ = 8.30 (bs, Ar*H*), 7.66 (bs, Ar*H*), 7.52 (bs, Ar*H*). ^{31}P{^{1}H} NMR (162 MHz, CD_2Cl_2, 25 °C): δ = 26.37 (s). ^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2): δ = -133.20 (s, 8F, *o*-C_6F_5), -163.59 (s, 4F, *p*-C_6F_5), -167.41 (s, 8F, *m*-C_6F_5). ^{11}B NMR (128 MHz, CD_2Cl_2): δ = -16.65 (bs). UV-vis: λ (nm): 384.0, 576.0, 722.0; ε (L mol^{-1} cm^{-1}): 650, 470, 80. Anal. Calc. for $C_{53}H_{24}BF_{20}O_3PV$: C, 53.88%; H, 2.05. Found: C, 54.48%, H, 2.45%.

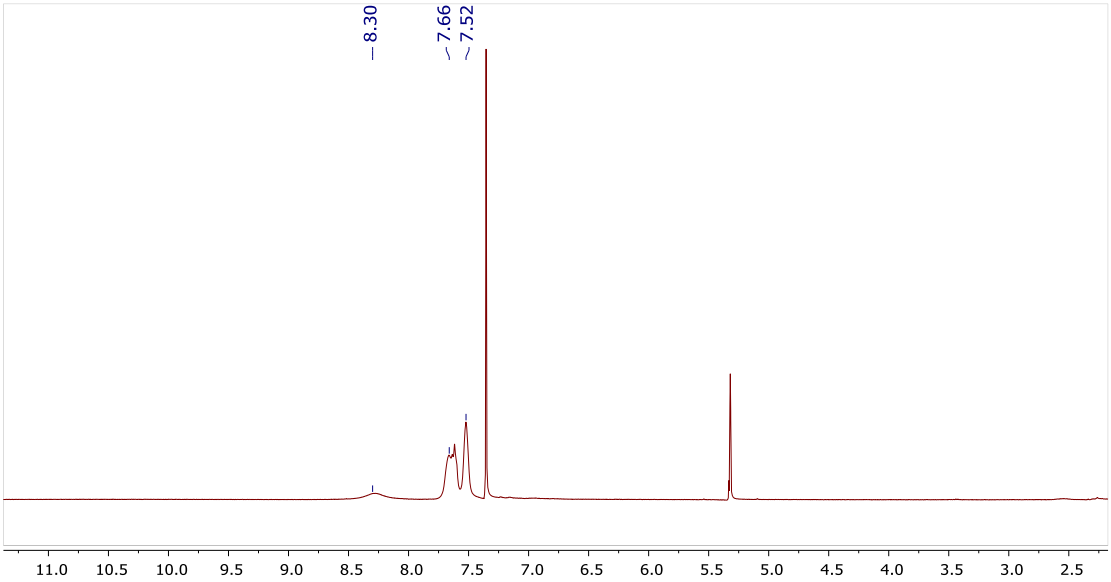


Figure S10: ^{1}H NMR spectrum of $[Ph_2P(O)(C_6H_4\text{-}p\text{-}COOVCp_2)][B(C_6F_5)_4]$ (**5**) (400 MHz, CD_2Cl_2, 25 °C).

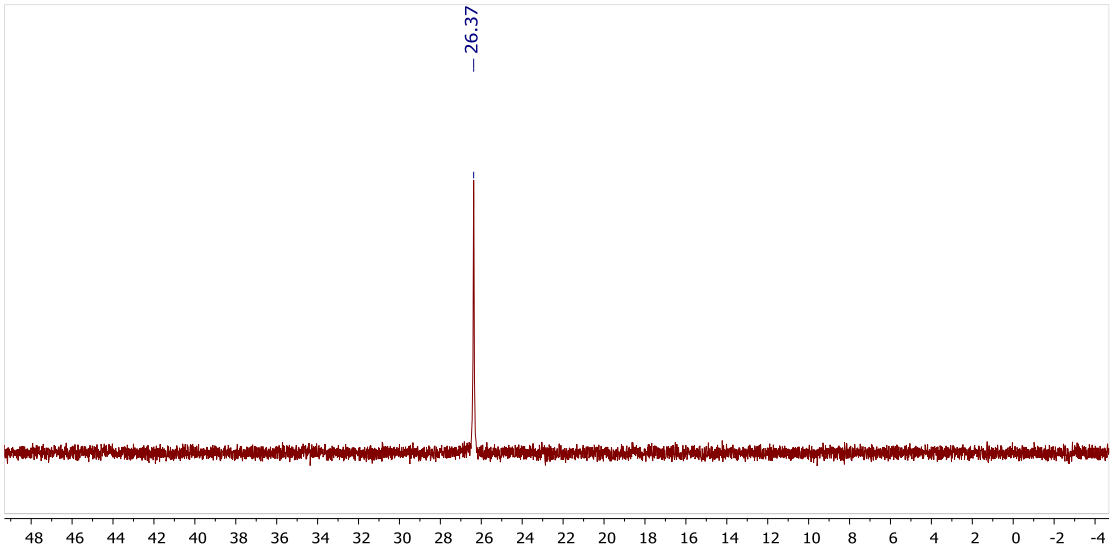


Figure S11: $^{31}P\{^{1}H\}$ NMR spectrum of $[Ph_2P(O)(C_6H_4\text{-}p\text{-}COOVCp_2)][B(C_6F_5)_4]$ (**5**) (162 MHz, CD_2Cl_2, 25 ºC).

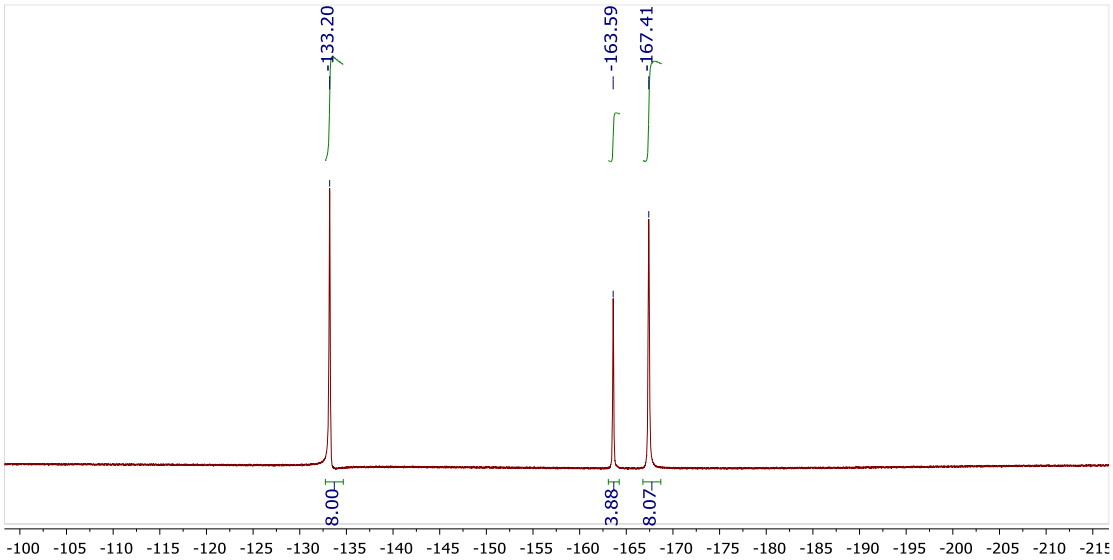


Figure S12: $^{19}F\{^{1}H\}$ NMR spectrum of $[Ph_2P(O)(C_6H_4\text{-}p\text{-}COOVCp_2)][B(C_6F_5)_4]$ (**5**) (376 MHz, CD_2Cl_2, 25 ºC).

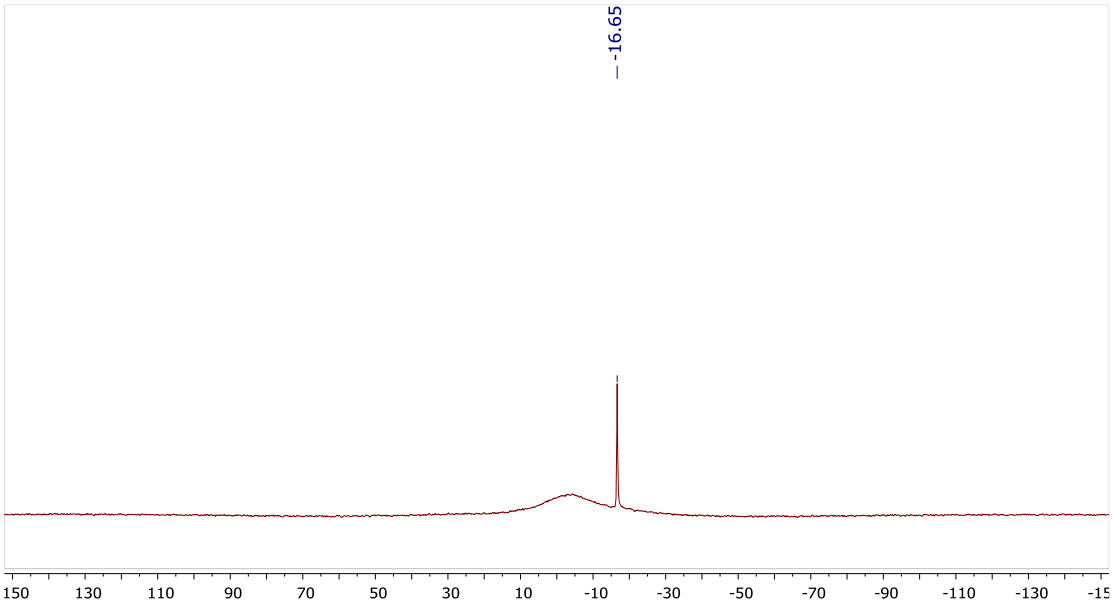


Figure S13: ^{11}B NMR of $[Ph_2P(O)(C_6H_4\text{-}p\text{-}COOVCp_2)][B(C_6F_5)_4]$ (**5**) (128 MHz, CD_2Cl_2, 25 ^oC).

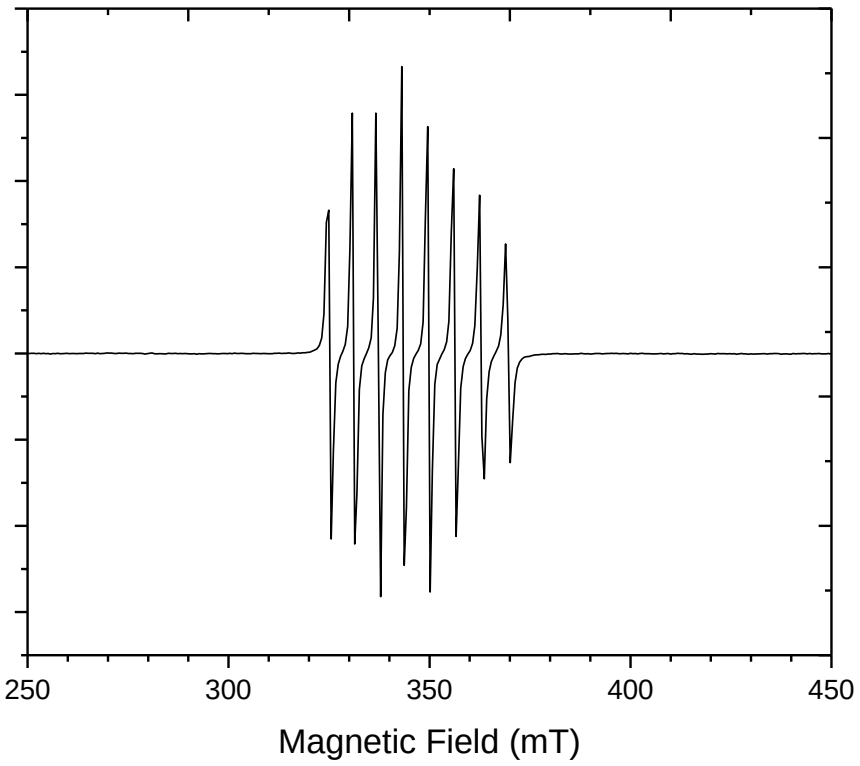


Figure S14: X-band EPR spectrum of **5** (DCM, 300 K).

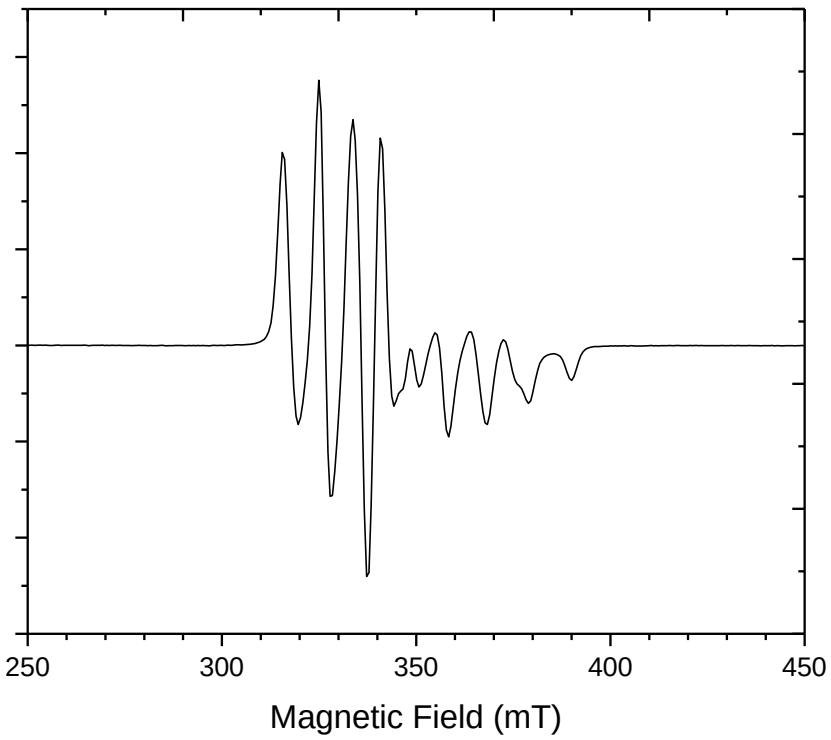


Figure S15: X-band EPR spectrum of **5** (DCM, 100 K).

3 Supplementary Figures for Cyclic Voltammetry

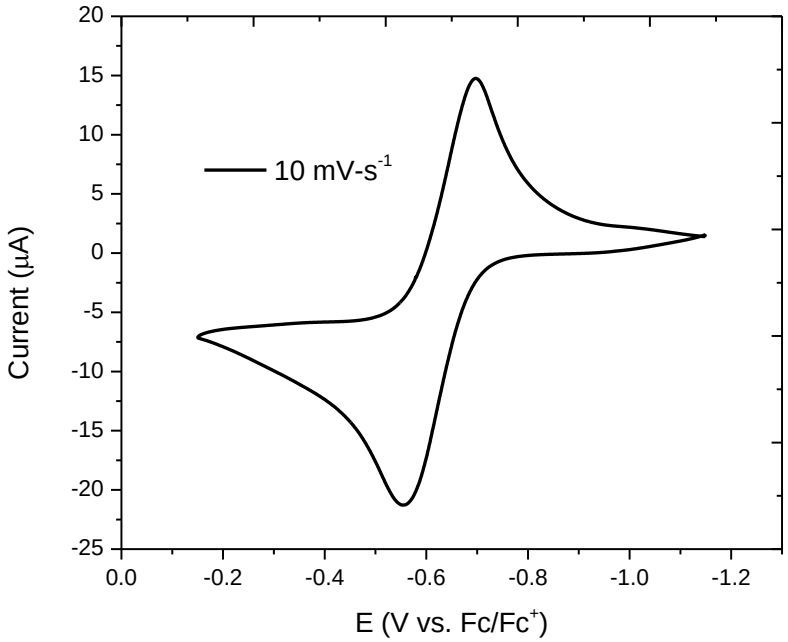


Figure S16: Cyclic voltammogram of **2** (2.3 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 10 mV-s^{-1}. Referenced to Fc/Fc^+.

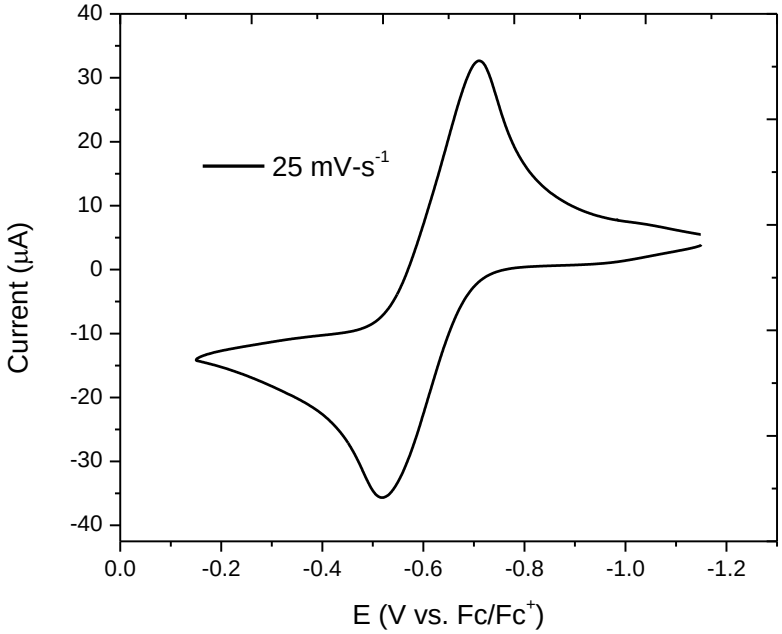


Figure S17: Cyclic voltammogram of **2** (2.3 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 25 mV-s^{-1}. Referenced to Fc/Fc^+.

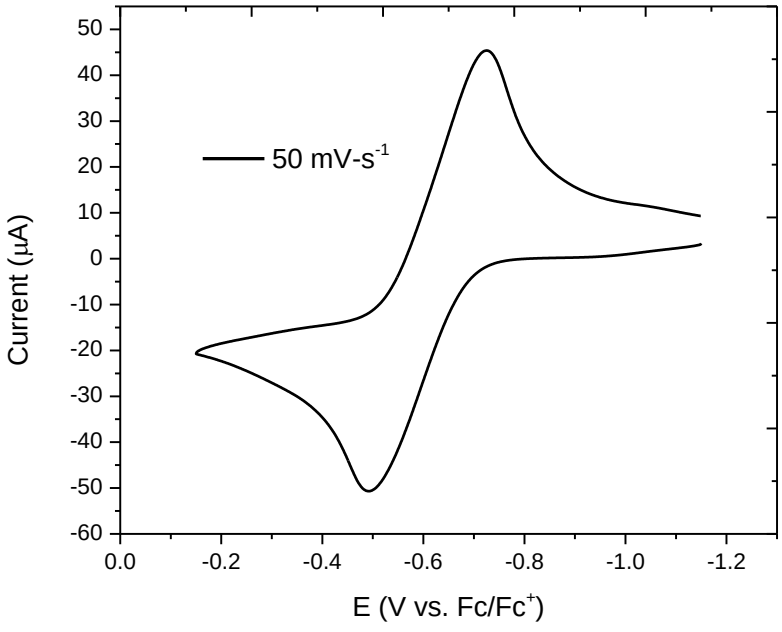


Figure S18: Cyclic voltammogram of **2** (2.3 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 50 mV-s^{-1}. Referenced to Fc/Fc^+.

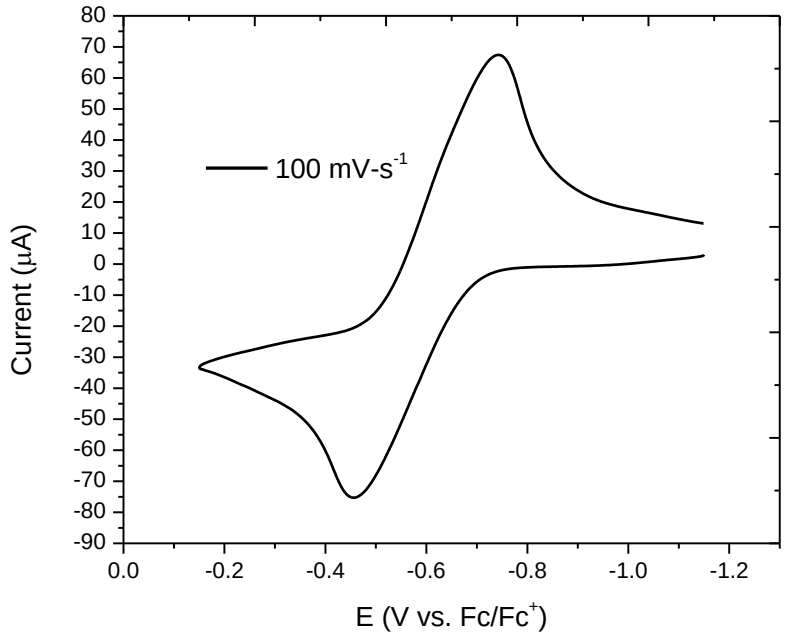


Figure S19: Cyclic voltammogram of **2** (2.3 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 100 mV-s^{-1}. Referenced to Fc/Fc^+.

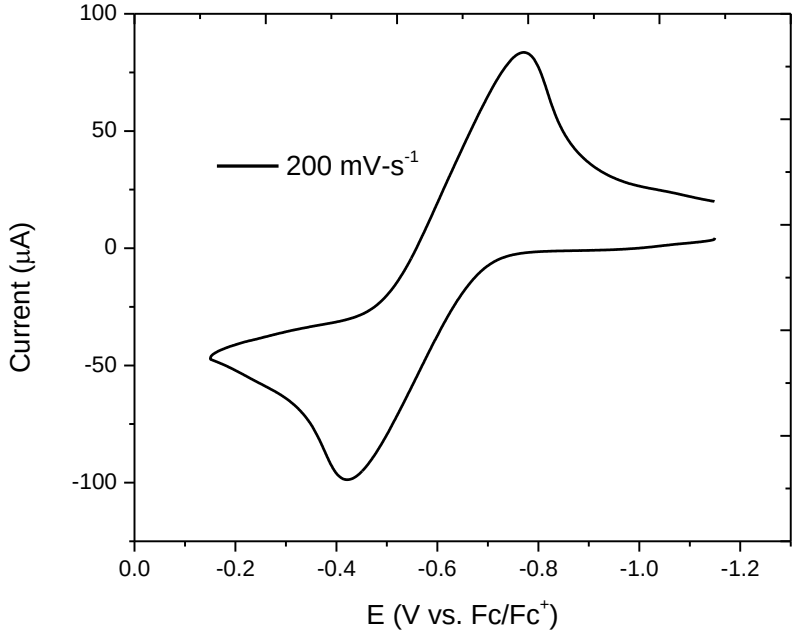


Figure S20: Cyclic voltammogram of **2** (2.3 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 200 mV-s^{-1}. Referenced to Fc/Fc^+.

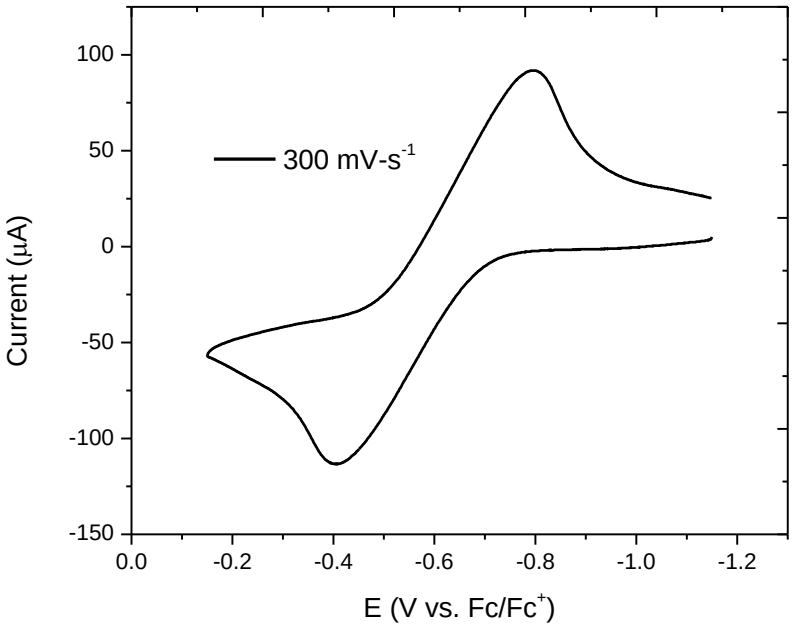


Figure S21: Cyclic voltammogram of **2** (2.3 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 300 mV-s^{-1}. Referenced to Fc/Fc^+.

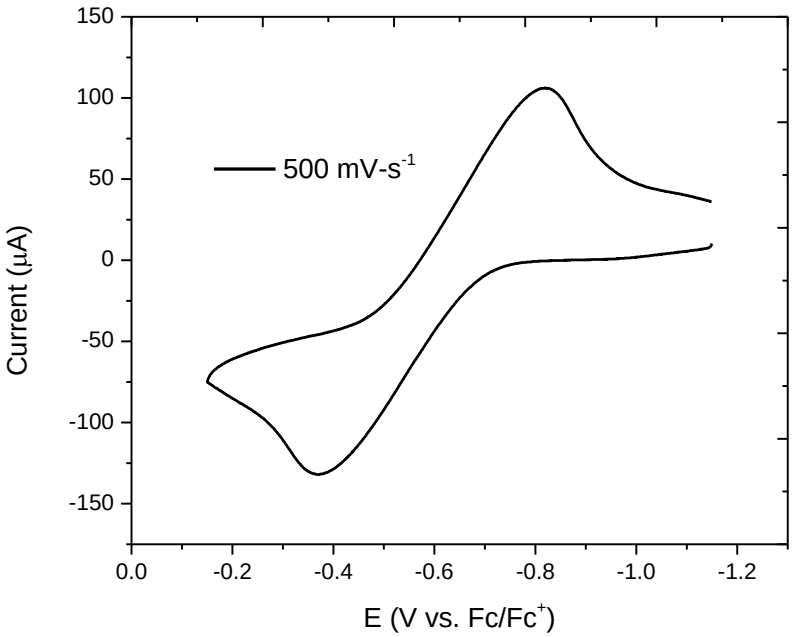


Figure S22: Cyclic voltammogram of **2** (2.3 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 500 mV-s^{-1}. Referenced to Fc/Fc^+.

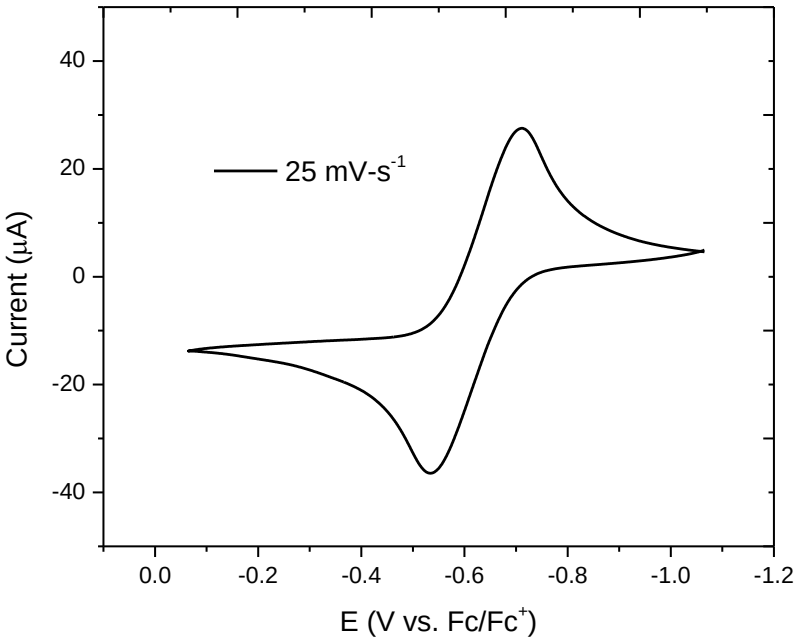


Figure S23: Cyclic voltammogram of **4** (3.6 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 25 mV-s^{-1}. Referenced to Fc/Fc^+.

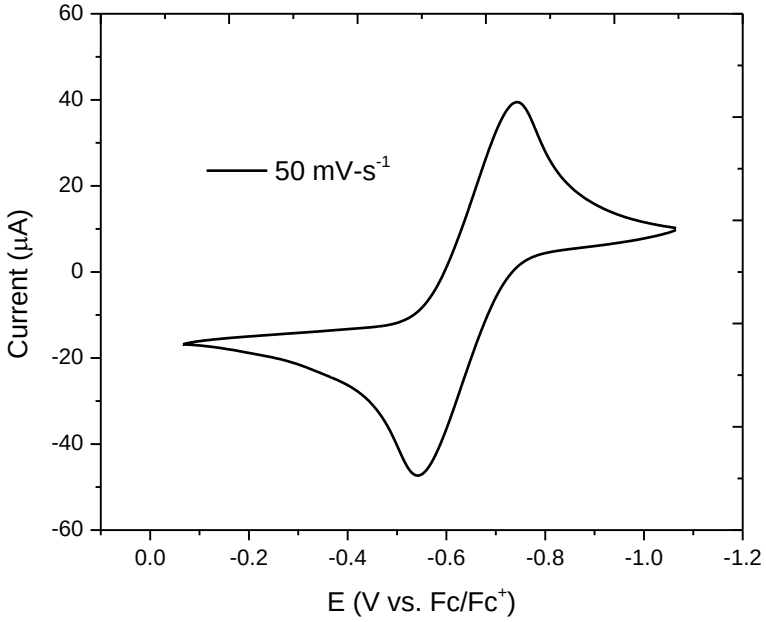


Figure S24: Cyclic voltammogram of **4** (3.6 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 50 mV-s^{-1}. Referenced to Fc/Fc^+.

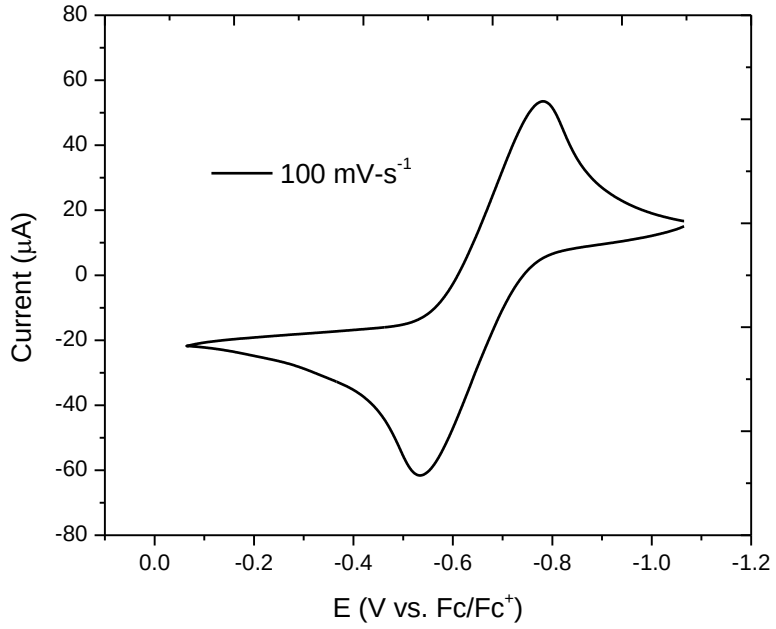


Figure S25: Cyclic voltammogram of **4** (3.6 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 100 mV-s^{-1}. Referenced to Fc/Fc^+.

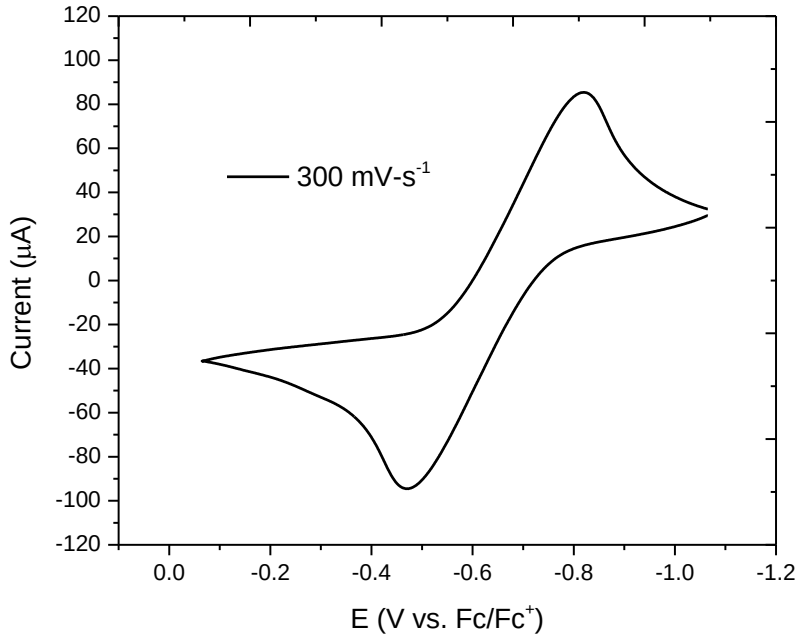


Figure S26: Cyclic voltammogram of **4** (3.6 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 300 mV-s^{-1}. Referenced to Fc/Fc^+.

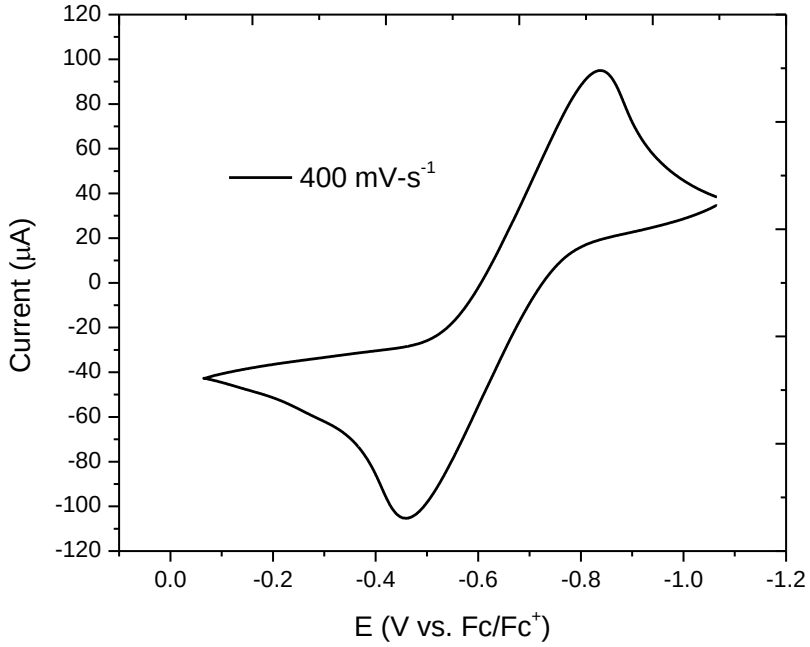


Figure S27: Cyclic voltammogram of **4** (3.6 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 400 mV-s^{-1}. Referenced to Fc/Fc^+.

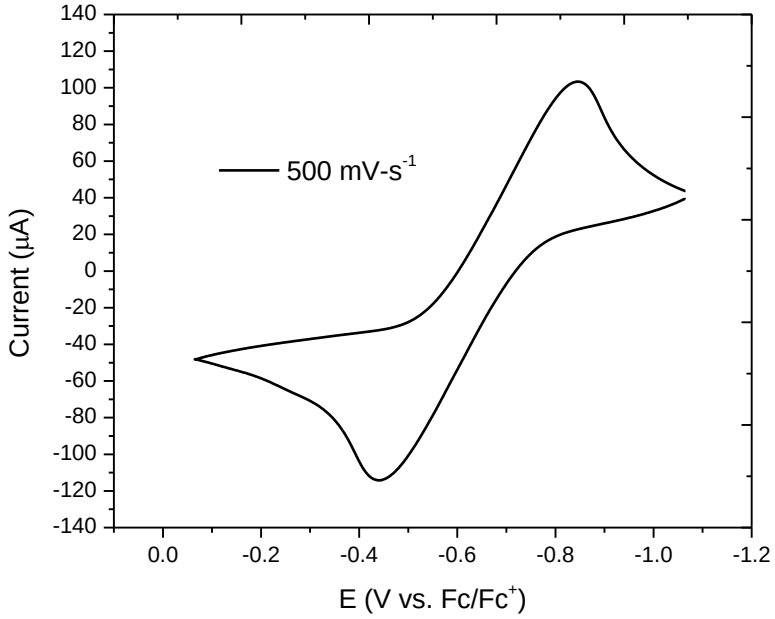


Figure S28: Cyclic voltammogram of **4** (3.6 mM) in 0.1 M $[Bu_4N][PF_6]$ supporting electrolyte in CH_2Cl_2 using a glassy carbon working electrode, platinum wire counter electrode, and Ag/Ag^+ pseudo-reference electrode. Scan rate: 500 mV-s^{-1}. Referenced to Fc/Fc^+.

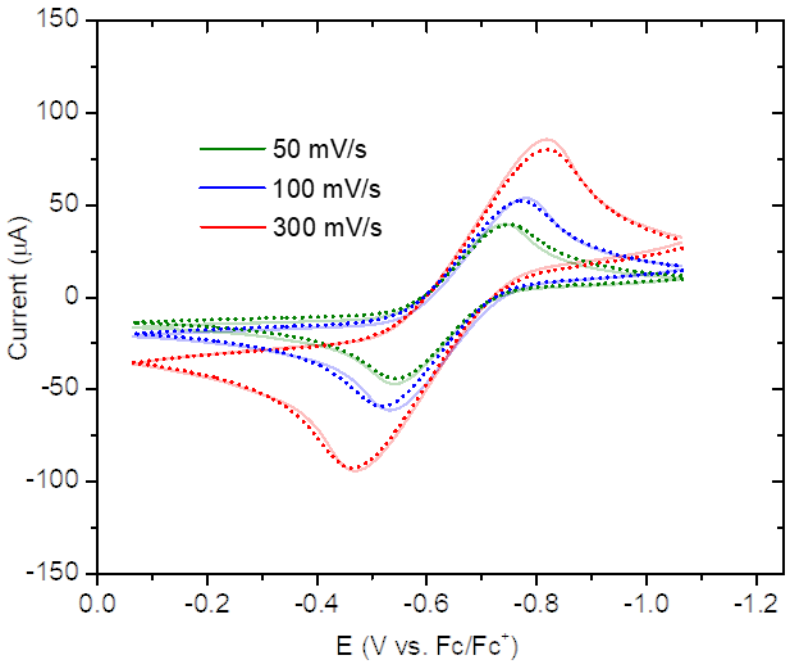


Figure S29: CVs of **4** (3.6 mM) in a 0.1 M [Bu_4N][PF_6] DCM solution at varying scan rates using a glassy carbon working electrode, platinum wire counter electrode, and referenced to the Fc/Fc^+ couple. The dotted traces represent the theoretical fit generated by DigiSim.

4. Supplementary Crystallographic Data

Table S1: Selected Bond Distances (Å) and Angles (°) for **2**, **4**, and **5**.

	2*	**4**	**5**
V1-O2	2.043	2.010(3)	2.075(2)
P1-O1	1.46(5)	1.482(3)	1.485(2)
O2-C1	1.26(2)	1.285(5)	1.275(4)
O3-C1	1.24(2)	1.220(6)	1.267(4)
V1-O2-C1	117.0(12)	119.0(3)	58.34(15)
O3-C1-O2	124.5(18)	125.7(4)	116.9(3)

* the bond lengths and angles are approximate due to the significant disorder in the structure arising from the perfect superposition of two molecules of **2** axially trans-disposed along the P=O bond vector.

Table S2. Crystallographic Data and Refinement for Complexes.

	2	**4**	**5**
Empirical formula	$C_{51}H_{33}O_7PV_3$	$C_{29}H_{24}O_3PV$	$C_{54}H_{24}BCl_2F_{20}O_3PV$
Formula weight	941.61	502.43	1264.40
Temperature (K)	100(2)	100(2)	100(2)
Crystal system	Hexagonal	Monoclinic	Monoclinic
Space group	P 63/mcm	P 21/c	C 2/c
a (Å)	15.033(2)	10.190(8)	25.0426(19)
b (Å)	15.033(2)	11.081(9)	33.159(2)
c (Å)	11.491(3)	21.340(19)	16.5246(11)
α (deg)	90.00	90.00	90.00
β (deg)	90.00	97.09(6)	115.089(4)
γ (deg)	120.00	90.00	90.00
Volume (Å^3)	2248.8(7)	2391(4)	12427.1(16)
Z	2	4	8
Dcalc (g/cm^3)	1.390	1.396	1.352
F(000)	960.5	1042.1	5041.9
θ Range (deg)	1.56-24.84	1.92-27.15	1.414-26.520
no. of rflns collected	11757	15809	36579
no. of unique rflns	733	5178	12740
no. of obsd rflns	582	2614	7822
no. of par.	61	307	739
Final R, R_w (I > 2σ(I))	0.1347, 0.2494	0.0639, 0.2280	0.0467, 0.1358
Goodness-of-fit on F^2	1.051	0.897	0.986

5. Supplementary Figures for FT-IR

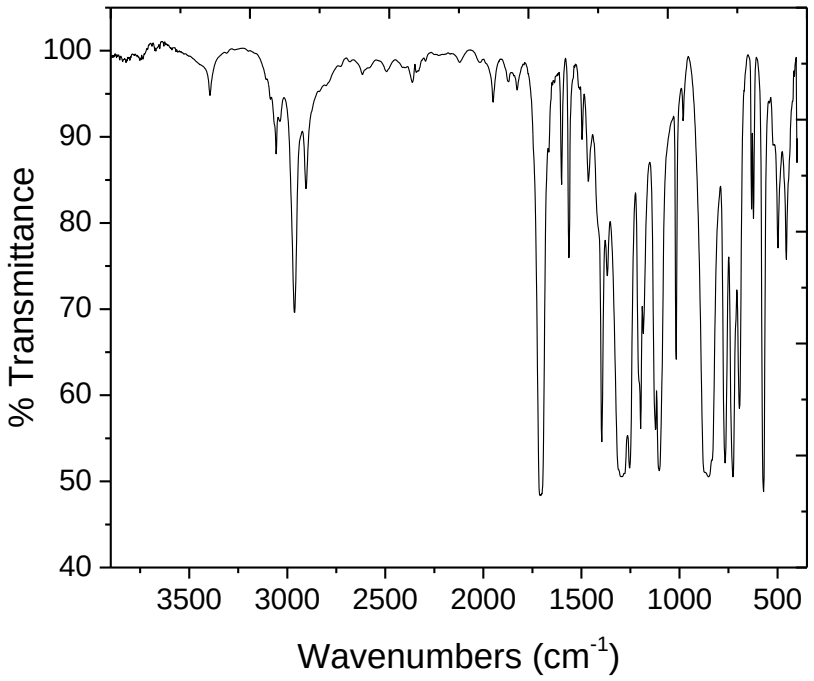


Figure S30: IR spectrum of P(O)(C_6H_4-*p*-$COOSiMe_3$)$_3$ (**1**) (KBr pellet).

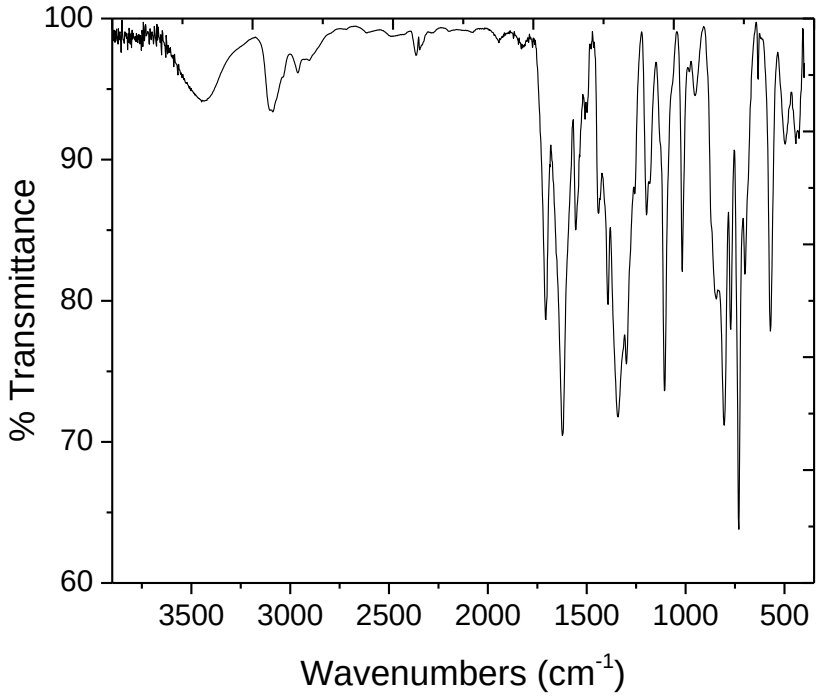


Figure S31: IR spectrum of P(O)(C_6H_4-*p*-$COOVCp_2$)$_3$ (**2**) (KBr pellet).

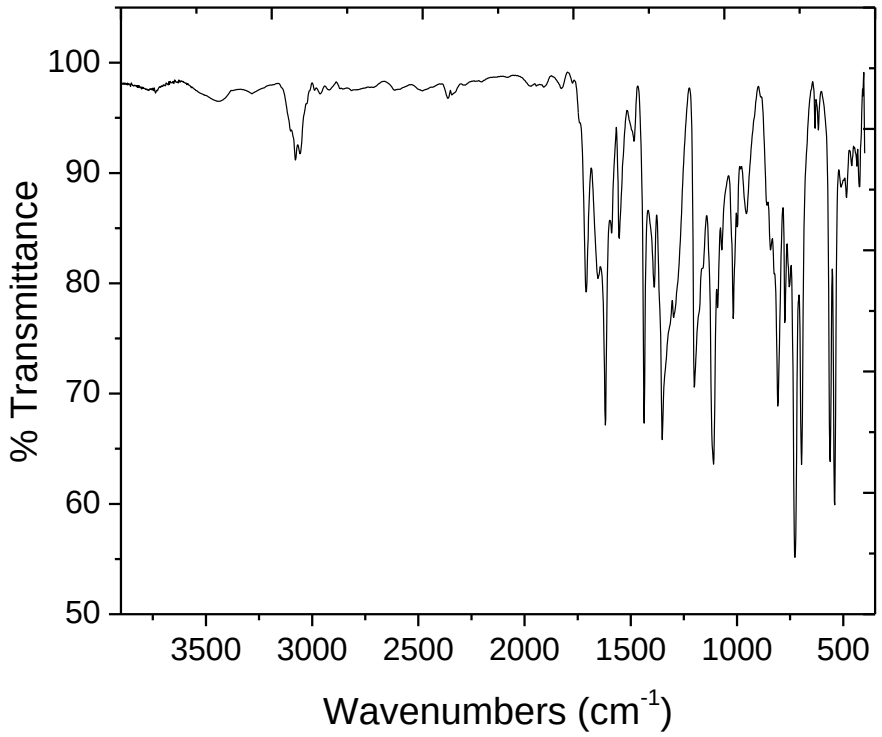


Figure S32: IR spectrum of $Ph_2P(O)(C_6H_4$-*p*-$COOVCp_2)$ (**4**) (KBr pellet).

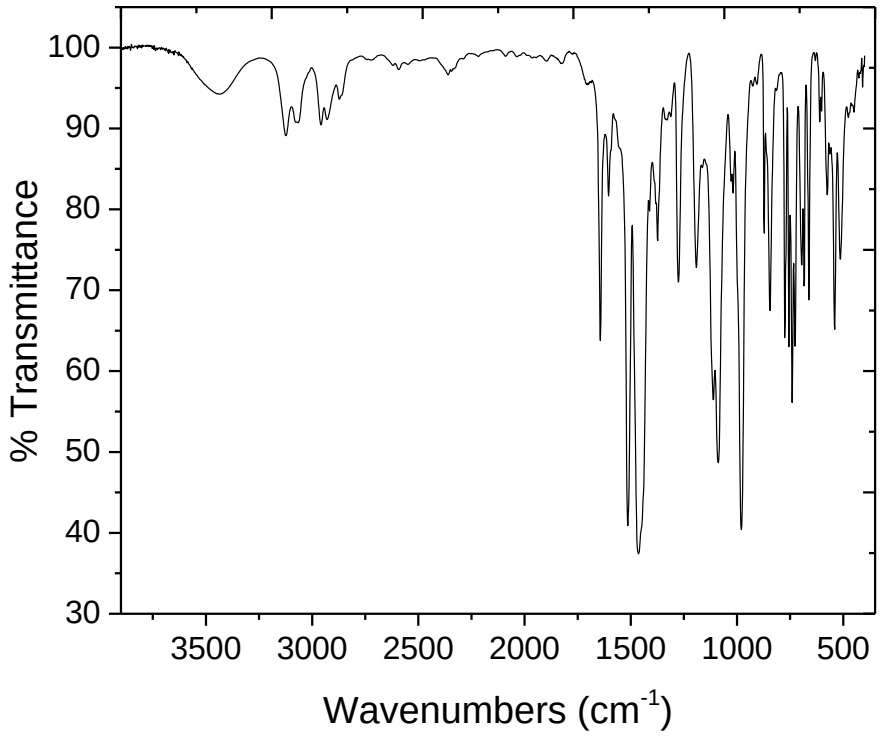


Figure S33: IR spectrum of $[Ph_2P(O)(C_6H_4$-*p*-$COOVCp_2)][B(C_6F_5)_4]$ (**5**) (KBr pellet).

6. Supplementary Figures for UV-Vis

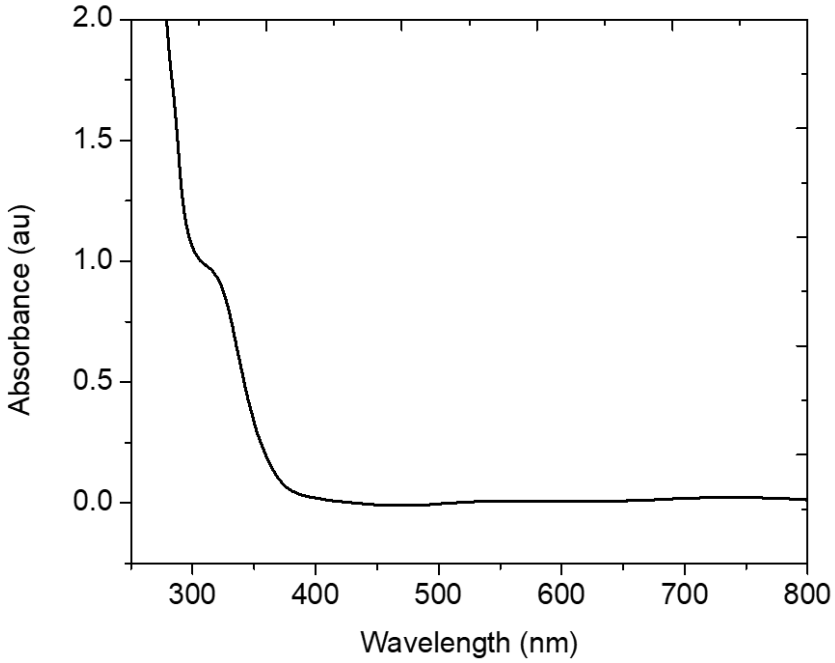


Figure S34: UV-Vis spectrum of $P(O)(C_6H_4\text{-}p\text{-}COOVCp_2)_3$ (**2**), $1x10^{-4}$ M in DCM.

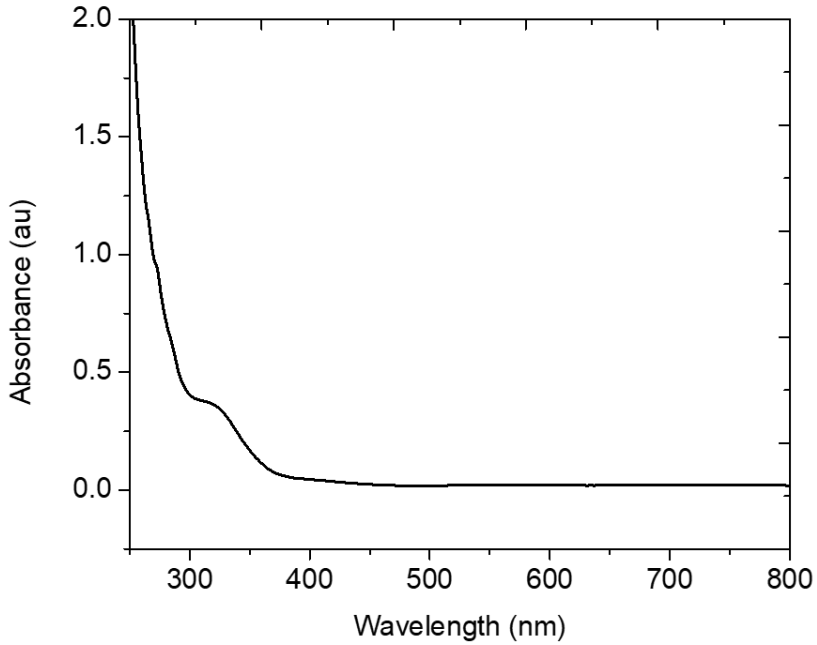


Figure S35: UV-Vis spectrum of $Ph_2P(O)(C_6H_4\text{-}p\text{-}COOVCp_2)$ (**4**), $1x10^{-4}$ M in DCM.

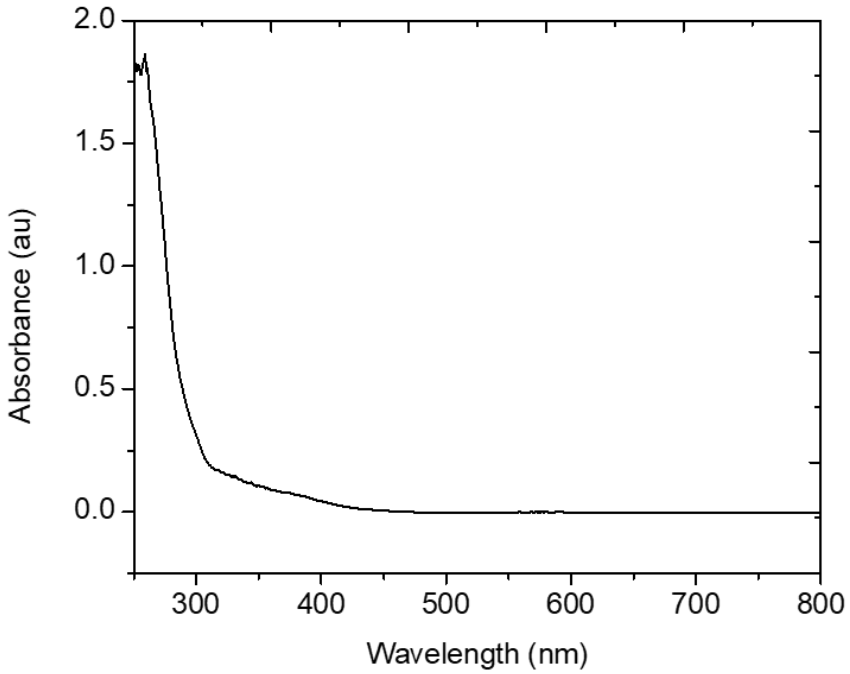


Figure S36: UV-Vis spectrum of $[Ph_2P(O)(C_6H_4$-*p*-$COOVCp_2)][B(C_6F_5)_4]$ (**5**), $1x10^{-4}$ M in DCM.

7. DFT calculations

DFT calculations were performed using Gaussian 09.2 Geometry optimization of all the molecules were carried out using the uwB97XD method with Ahlrichs' def2-SVP basis set, and with the relativistic effect of vanadium, which was accounted for by the Stuttgart-Dresden ECP, implemented in the Gaussian 09 software.[5-8] Compound **2** was calculated in the triplet state. Due to convergence problems with the wB97XD method, the TPPO, Me_3P=O and TPPO-$OPMe_3$ were calculated at the BP86-D3/def2-SVP level of theory. Thermal energy corrections were extracted from the results of frequency analysis performed at the same level of theory. Frequency analysis of all the molecules and intermediates contained no imaginary frequency showing that these are energy minima.

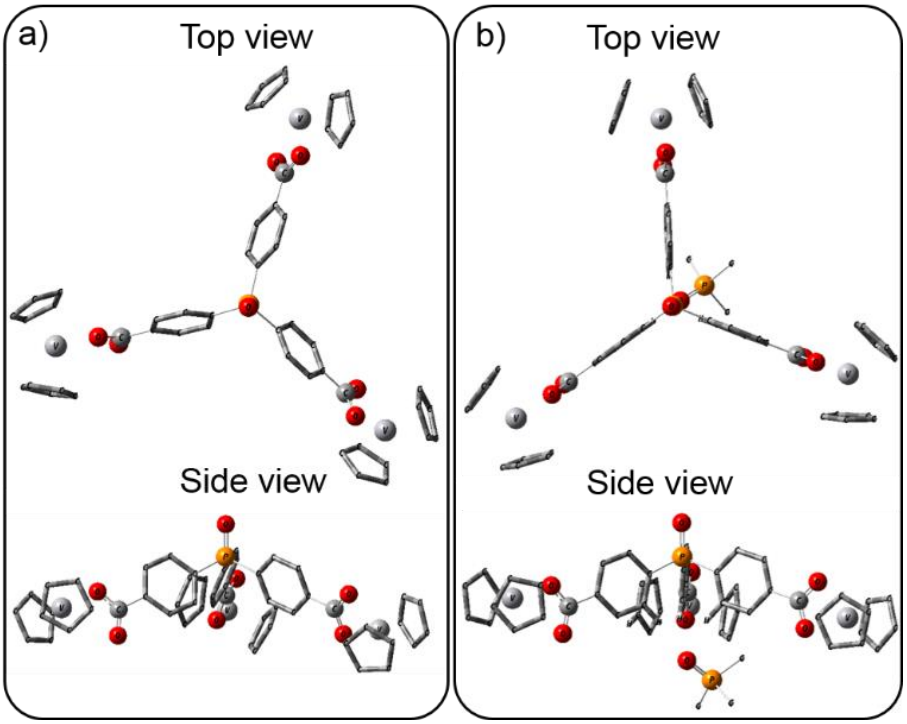


Figure S37: a) Optimized structure of **2**. b) Optimized structure of **2**·$OPMe_3$. Non-relevant hydrogen atoms were omitted for clarity.

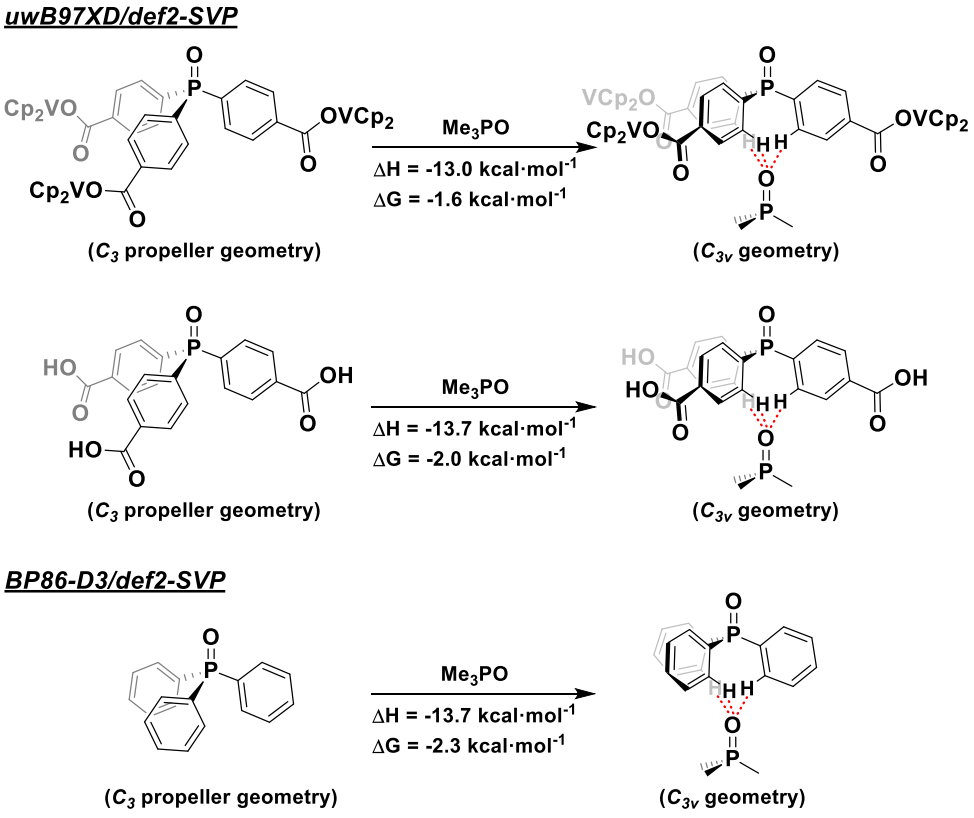
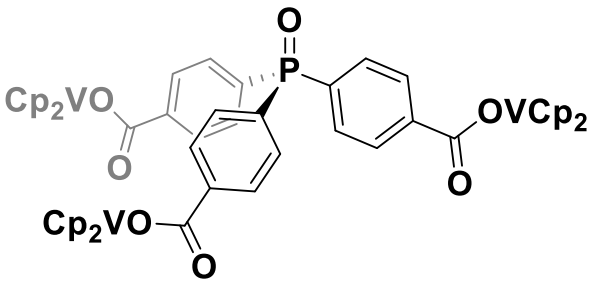


Figure S38. Calculated thermodynamic values using the respective levels of theory. A different level of theory was utilized for TPPO (bottom) due to convergence problems. Calculated coordinates for individual species are shown below.

uwB97XD/def2-SVP SDD(V)



(C_3 propeller geometry)

P	-0.10637300	-0.09683400	2.22609500
C	5.88121100	-7.30164600	-2.24394800
H	6.71585600	-7.34493900	-2.94131300
C	4.73519600	-6.50660300	-2.38740700
H	4.51517200	-5.82774700	-3.20759000
C	3.94123100	-6.70054500	-1.22088800
H	2.98757500	-6.22005000	-1.01820100
C	4.59094200	-7.64439400	-0.37441600
H	4.23900900	-7.98780200	0.59518600
C	5.79213300	-8.00234800	-1.00439600
H	6.54497700	-8.67622400	-0.59974400
V	5.78581600	-5.74155000	-0.54103900
C	4.08428500	-4.06821100	0.24716500
O	4.60155500	-3.97148200	-0.89757100
C	3.07307200	-3.07675300	0.71543200
C	2.73288100	-1.99242200	-0.09860000
H	3.22264100	-1.88325800	-1.06755200
C	1.78879500	-1.06787900	0.33573900
H	1.54655000	-0.20911000	-0.29522100
C	1.16845800	-1.23025900	1.58006100
C	1.52212900	-2.30732300	2.40012400
H	1.05184600	-2.40352200	3.38141500
C	2.47170600	-3.22812200	1.96798800
H	2.76145700	-4.07355600	2.59444100
O	-0.19867800	-0.12293500	3.72183000
O	4.43919900	-5.02688200	0.98322300
C	1.62407300	5.40886900	0.24162700
O	1.36257300	5.81182800	-0.92316200
C	1.16957700	4.06711000	0.70865300
C	0.40630000	3.25602200	-0.13568900

H	0.14548100	3.62490100	-1.12905200
C	-0.01365000	2.00194700	0.29754000
H	-0.62783300	1.38202700	-0.35995800
C	0.33794700	1.54798400	1.57396100
C	1.08526200	2.37036100	2.42513100
H	1.32389000	2.01627800	3.43068100
C	1.50149000	3.62521500	1.99274600
H	2.08703500	4.27869200	2.64164900
O	2.28239000	6.16767700	1.00156800
C	-5.46216100	-1.52155800	-0.37253200
O	-5.51743700	-1.84699300	-1.55396500
C	-4.14117900	-1.18690800	0.27230700
C	-2.96648400	-1.37864800	-0.46026000
H	-3.04554100	-1.77395400	-1.47444400
C	-1.73157600	-1.07978300	0.10536300
H	-0.81885700	-1.26174100	-0.46716300
C	-1.66215800	-0.56553300	1.40593100
C	-2.83682400	-0.38430300	2.14420400
H	-2.76708900	-0.00975500	3.16818800
C	-4.07037000	-0.69573100	1.57876000
H	-4.99482300	-0.56505200	2.14323400
O	-6.49127500	-1.44073500	0.40130300
C	3.82803400	8.49400500	-2.12877400
H	3.53789500	9.27844300	-2.82522000
C	3.63056900	7.11774200	-2.31903400
H	3.17197100	6.64157800	-3.18206600
C	4.09661500	6.46299500	-1.14256400
H	4.07685500	5.39077200	-0.96522600
C	4.60780100	7.44296100	-0.24430400
H	5.01255000	7.25651000	0.74732900
C	4.42909400	8.69400000	-0.85084100
H	4.66988600	9.65679800	-0.40404800
V	2.37832000	7.67642600	-0.53480300
C	-9.49358600	-0.76330700	-1.98555100
H	-9.93431100	-1.32275300	-2.80873100
C	-8.21718100	-0.15161000	-1.98713600
H	-7.48341100	-0.18291200	-2.78906800
C	-8.03560700	0.45351800	-0.72227400
H	-7.13358800	0.95984800	-0.38747800

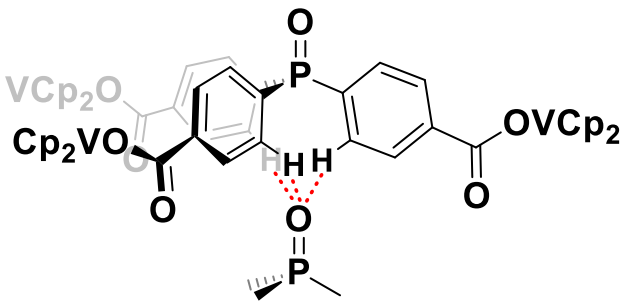
C	-9.18487300	0.21707000	0.06936900
H	-9.33585100	0.54359900	1.09662000
C	-10.09278000	-0.53410100	-0.71702800
H	-11.07466500	-0.88255500	-0.40151600
V	-8.27322600	-1.83051000	-0.41074100
C	-9.69560200	-3.57700900	-0.74226300
H	-10.64169300	-3.44426300	-1.26317000
C	-8.45573800	-3.92220900	-1.34032800
H	-8.27165600	-4.06827700	-2.40315800
C	-7.48946500	-3.98408800	-0.31905700
H	-6.42873000	-4.17266700	-0.46500700
C	-8.12864900	-3.68380600	0.91839400
H	-7.63492200	-3.60883400	1.88483300
C	-9.49171300	-3.44035600	0.65746100
H	-10.24835400	-3.16431700	1.39026900
C	1.75626100	9.78043400	-0.59356900
H	2.39332100	10.56323300	-0.99703200
C	0.78390100	9.04137800	-1.32996300
H	0.56460600	9.13183200	-2.39120500
C	0.12504300	8.20102200	-0.40765200
H	-0.63481600	7.46406700	-0.65565800
C	0.69459600	8.39487500	0.86877000
H	0.44061300	7.83632400	1.76642400
C	1.71785600	9.36511400	0.76897900
H	2.32719000	9.74578100	1.58503100
C	7.74050600	-4.89138600	-1.22686500
H	7.94685900	-4.66367900	-2.26990200
C	7.26555000	-3.98870300	-0.25065200
H	6.95932800	-2.96195700	-0.43556700
C	7.15368300	-4.66891000	0.98066400
H	6.74605500	-4.25158100	1.89821500
C	7.55769500	-6.00986400	0.79774100
H	7.60270900	-6.77954300	1.56448200
C	7.94219800	-6.14002300	-0.56891600
H	8.36390000	-7.03204300	-1.02471300

Sum of electronic and zero-point Energies = -3048.434188

Sum of electronic and thermal Energies = -3048.380017

Sum of electronic and thermal Enthalpies = -3048.379073

Sum of electronic and thermal Free Energies = -3048.531550



(C_{3v} geometry)

P	0.40034400	-0.03388500	-2.17365700
C	-4.33640500	-8.76455000	1.04872900
H	-5.04630300	-9.10204700	1.80141800
C	-3.20832700	-7.96216400	1.28806300
H	-2.87659900	-7.57521500	2.24826500
C	-2.59950000	-7.71672300	0.02343500
H	-1.70680400	-7.11964400	-0.14421500
C	-3.34093500	-8.39794700	-0.98311600
H	-3.14214500	-8.37271000	-2.05175400
C	-4.41697200	-9.03257900	-0.35034600
H	-5.20635000	-9.59429700	-0.84665600
V	-4.55980400	-6.74356300	-0.01758300
C	-3.08245300	-4.80293900	-0.61782500
O	-3.34119600	-5.07332200	0.58729800
C	-2.21927100	-3.64197200	-0.97204400
C	-1.66186900	-2.85602300	0.04113200
H	-1.86260400	-3.12160900	1.08080900
C	-0.86386500	-1.76152800	-0.27323900
H	-0.45352200	-1.16259100	0.54307700
C	-0.61538800	-1.44773700	-1.61482400
C	-1.16352400	-2.23921000	-2.62998700
H	-0.94787900	-1.98200400	-3.66952500
C	-1.96494000	-3.33231100	-2.31002100
H	-2.40065800	-3.95742500	-3.09136000
O	0.54813400	-0.03602800	-3.66907600
O	-3.57862500	-5.54120100	-1.50990000
C	-2.54972000	5.07304700	-0.59206600

O	-2.70447800	5.41363600	0.61291100
C	-1.81903500	3.82503800	-0.94796000
C	-1.32614600	2.99254300	0.06146500
H	-1.47680200	3.28232600	1.10343000
C	-0.65194500	1.81883700	-0.25857700
H	-0.29720900	1.18422000	0.55698200
C	-0.45769800	1.47596500	-1.60210800
C	-0.93826000	2.31503900	-2.61356800
H	-0.76406900	2.03398200	-3.65465800
C	-1.62130000	3.48372500	-2.28799600
H	-2.00596000	4.14579500	-3.06566500
O	-3.03164500	5.82049800	-1.48479500
C	5.97296400	-0.34039800	0.34104400
O	6.14219100	-0.30811200	1.55501000
C	4.59178400	-0.27141500	-0.25736600
C	3.48125900	-0.21976100	0.58991100
H	3.64441200	-0.23491700	1.66872600
C	2.19296000	-0.14912700	0.06868500
H	1.35745400	-0.11207500	0.77164900
C	2.00825600	-0.12694800	-1.32144700
C	3.11914300	-0.17804000	-2.17176000
H	2.95543500	-0.15949500	-3.25149100
C	4.40385800	-0.25137200	-1.64128400
H	5.27627700	-0.29222200	-2.29505100
O	6.93573500	-0.42352400	-0.51732400
C	-5.68824400	7.77714900	1.10245100
H	-5.70882100	8.54530300	1.87306000
C	-5.40233200	6.41857400	1.30922900
H	-5.17277900	5.94120200	2.25847300
C	-5.42334800	5.79014000	0.03062700
H	-5.23188900	4.73759600	-0.16137200
C	-5.75376200	6.76416800	-0.95398700
H	-5.81966900	6.59509800	-2.02593300
C	-5.90461300	7.98974700	-0.29135300
H	-6.10690100	8.94868000	-0.76497000
V	-3.74782200	7.19778700	0.00379700
C	10.17051500	1.05955200	1.14220400
H	10.85125100	0.74373900	1.93064400
C	8.84890000	1.53588100	1.32619600

H	8.31580300	1.62348800	2.27017400
C	8.31951900	1.81823900	0.04903000
H	7.30535100	2.15326400	-0.15405900
C	9.29789200	1.51551800	-0.93130000
H	9.17465900	1.61112400	-2.00829800
C	10.44926500	1.05135800	-0.25187500
H	11.38001600	0.72971800	-0.71610900
V	8.80750500	-0.44399500	0.14612000
C	10.47867500	-1.93290900	0.54781400
H	11.49799900	-1.60057600	0.73400100
C	9.47418400	-2.13279100	1.53124600
H	9.57840600	-1.95301200	2.59992800
C	8.30273800	-2.55592900	0.87271100
H	7.33764500	-2.73333800	1.34158100
C	8.58473900	-2.62711900	-0.52153400
H	7.86479400	-2.87272100	-1.29878200
C	9.92595100	-2.24752200	-0.72273100
H	10.43948900	-2.17765500	-1.68038000
C	-3.40213400	9.33645800	0.33921400
H	-4.20778600	10.02591500	0.57781100
C	-2.60371100	8.63328400	1.28910800
H	-2.70514200	8.66015800	2.37150100
C	-1.62031700	7.93340100	0.55672200
H	-0.88550200	7.25037600	0.97603500
C	-1.81992900	8.17749400	-0.81866200
H	-1.26225300	7.71631200	-1.63015300
C	-2.93073500	9.03712500	-0.97214200
H	-3.32145700	9.42529700	-1.90972800
C	-6.34540400	-6.30574000	1.28168500
H	-6.33400700	-6.45003700	2.35956400
C	-6.08487100	-5.10153600	0.59596600
H	-5.75081000	-4.17336000	1.05300500
C	-6.21361600	-5.33244300	-0.79015600
H	-6.00385100	-4.60827300	-1.57356300
C	-6.56554500	-6.68686300	-0.99609300
H	-6.75993600	-7.16413500	-1.95346100
C	-6.66643200	-7.28330600	0.29326000
H	-6.97959700	-8.30487900	0.49237000
O	-0.20566700	0.00520000	2.37764200

P	-1.49861400	0.00425100	3.15250600
C	-1.59447200	1.35778000	4.35617900
H	-0.74827600	1.27526000	5.05292200
H	-1.51009800	2.31426200	3.82048000
H	-2.53885200	1.33730200	4.91885400
C	-1.74366500	-1.51959000	4.10581700
H	-0.89430800	-1.64943000	4.79131200
H	-2.68110300	-1.49592000	4.67982700
H	-1.76384000	-2.37323000	3.41337400
C	-2.97656900	0.17107600	2.11321700
H	-3.89545800	0.15407400	2.71716500
H	-2.92102600	1.11729900	1.55615600
H	-2.99955600	-0.65282700	1.38541900

Sum of electronic and zero-point Energies = -3584.374520

Sum of electronic and thermal Energies = -3584.311126

Sum of electronic and thermal Enthalpies = -3584.310181

Sum of electronic and thermal Free Energies = -3584.483783

uwB97XD/def2-SVP

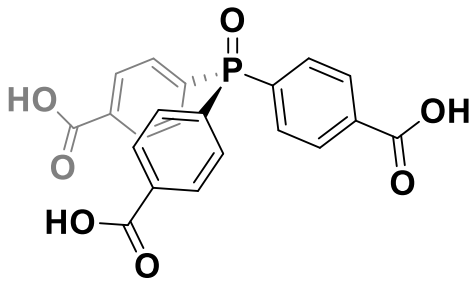
O	-0.00053200	-0.00303200	1.67849900
P	-0.00020600	-0.00060200	0.18413000
C	-1.52474900	-0.66491800	-0.55698900
H	-1.66440500	-1.69870100	-0.20941600
H	-2.37674200	-0.06697000	-0.20281800
H	-1.49529500	-0.64744100	-1.65626200
C	1.34000300	-0.98546800	-0.55669100
H	1.25161300	-2.02247200	-0.20191800
H	1.31057900	-0.96918000	-1.65598000
H	2.30341400	-0.58573400	-0.20895400
C	0.18546900	1.65375500	-0.55301400
H	0.18799800	1.62161200	-1.65235700
H	-0.64219200	2.28891400	-0.20597800
H	1.12803400	2.09304600	-0.19610400

Sum of electronic and zero-point Energies = -535.918963

Sum of electronic and thermal Energies = -535.911313

Sum of electronic and thermal Enthalpies = -535.910369

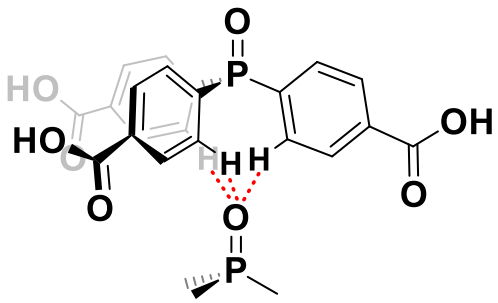
Sum of electronic and thermal Free Energies = -535.949759



(C_3 propeller geometry)

P	0.00378800	-0.00187600	1.38550700
C	-3.67414600	-4.38733400	-0.73076400
C	-2.73198500	-3.32441200	-0.26798200
C	-1.65769900	-2.89463500	-1.05321700
H	-1.48712700	-3.34675900	-2.03067600
C	-0.80702100	-1.90019700	-0.57877000
H	0.04279600	-1.58395300	-1.18858000
C	-1.02998700	-1.32648800	0.67753600
C	-2.09543600	-1.77079900	1.46885100
H	-2.23949900	-1.33780700	2.46129900
C	-2.94550200	-2.76344600	0.99473000
H	-3.78310600	-3.12337600	1.59481800
O	0.00478200	-0.00156400	2.88260600
O	-4.61185400	-4.78877200	-0.09259200
C	5.64294600	-0.97620400	-0.73268200
C	4.24961900	-0.69919300	-0.27033200
C	3.33690700	0.01077600	-1.05659800
H	3.64136800	0.38504300	-2.03445800
C	2.04967200	0.24545100	-0.58179800
H	1.34874600	0.81962700	-1.19241800
C	1.66714600	-0.23352000	0.67577000
C	2.58788800	-0.92892900	1.46793100
H	2.28758700	-1.26859000	2.46178300
C	3.87322800	-1.16438500	0.99319700
H	4.60655300	-1.70554500	1.59372900

O	6.46239900	-1.58383600	-0.09478900
C	-1.97668600	5.36849000	-0.73040100
C	-1.51951700	4.02361200	-0.26792800
C	-1.67758500	2.87807600	-1.05423700
H	-2.15403100	2.95490600	-2.03201800
C	-1.23599600	1.64625300	-0.57995600
H	-1.38244000	0.75177000	-1.19025700
C	-0.62902500	1.55457600	0.67716900
C	-0.48753700	2.69969500	1.46937700
H	-0.04124600	2.60919900	2.46226800
C	-0.92753400	3.93029900	0.99518700
H	-0.82543300	4.83623200	1.59534600
O	-1.85966900	6.38222200	-0.09296400
O	-3.37337400	-4.86117300	-1.94701400
H	-4.03288500	-5.53826800	-2.15433900
O	5.90054900	-0.47539300	-1.94803800
H	6.81811300	-0.70221000	-2.15554900
O	-2.53867500	5.34129000	-1.94599100
H	-2.79999200	6.24956400	-2.15380300
Sum of electronic and zero-point Energies=			-1675.445863
Sum of electronic and thermal Energies=			-1675.420782
Sum of electronic and thermal Enthalpies=			-1675.419838
Sum of electronic and thermal Free Energies=			-1675.505635



(C_{3v} geometry)

P	0.72278000	0.04991400	-1.94470900
C	-2.59335000	-4.97222400	-0.90767800
C	-1.78766000	-3.73010000	-1.08958500
C	-1.38858800	-2.93985700	-0.00616900
H	-1.66502300	-3.23866600	1.00610100
C	-0.63650500	-1.78815400	-0.21479200
H	-0.34877000	-1.18894300	0.65263400

C	-0.27380300	-1.42266700	-1.51635100
C	-0.66575600	-2.21622400	-2.59995400
H	-0.36126400	-1.92009900	-3.60626200
C	-1.42292600	-3.36421400	-2.38727700
H	-1.73742300	-3.99459600	-3.22095700
O	1.04957300	0.07078800	-3.40986500
O	-2.95518400	-5.69051600	-1.80272700
C	-2.52014300	5.07976200	-0.73657800
C	-1.73543400	3.83129100	-0.96140800
C	-1.38314700	2.97747200	0.08946300
H	-1.67951700	3.22785600	1.10948300
C	-0.64955800	1.82190500	-0.15985600
H	-0.39963400	1.17449100	0.68436600
C	-0.25607000	1.51844100	-1.46829700
C	-0.60247900	2.37458700	-2.51940500
H	-0.27789600	2.12360300	-3.53167800
C	-1.34285400	3.52536100	-2.26663600
H	-1.62299000	4.20456700	-3.07373200
O	-2.84538200	5.84908800	-1.60303000
C	5.99179100	-0.07003400	1.12883400
C	4.66436400	-0.03728700	0.44799200
C	3.46319300	-0.01474900	1.16403500
H	3.47988900	-0.01967500	2.25426000
C	2.24471400	0.01383800	0.49240400
H	1.33219900	0.02969300	1.09280200
C	2.22554300	0.01931900	-0.90886900
C	3.42851300	-0.00201500	-1.62515800
H	3.39138900	0.00423200	-2.71675500
C	4.64321300	-0.03041400	-0.94894800
H	5.59047400	-0.04795200	-1.49080500
O	7.05181600	-0.09064100	0.55809100
O	-0.35267800	0.00589200	2.49574900
P	-1.70932400	-0.09706300	3.14743900
C	-2.00589200	1.22111900	4.35624100
H	-1.21862800	1.18366800	5.12237800
H	-1.94381600	2.19196800	3.84409400
H	-2.99070700	1.12270500	4.83495300
C	-1.93505200	-1.65343900	4.05043500
H	-1.14109700	-1.74291300	4.80529400

H	-2.91752400	-1.70347900	4.54117000
H	-1.83827100	-2.49111700	3.34526900
C	-3.08828500	-0.00508600	1.97198800
H	-4.05829300	-0.09007600	2.48284100
H	-3.04031400	0.95241900	1.43366400
H	-2.99062600	-0.81521900	1.23481200
O	5.89850100	-0.07486400	2.46633800
H	6.80439600	-0.09589600	2.80537400
O	-2.88890000	-5.22458300	0.37734500
H	-3.40092300	-6.04555300	0.38485000
O	-2.84188000	5.27497700	0.55191700
H	-3.33738300	6.10529900	0.58775600

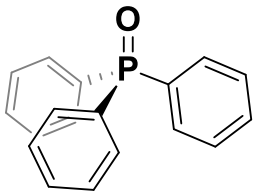
Sum of electronic and zero-point Energies= -2211.387200

Sum of electronic and thermal Energies= -2211.352997

Sum of electronic and thermal Enthalpies= -2211.352052

Sum of electronic and thermal Free Energies= -2211.458530

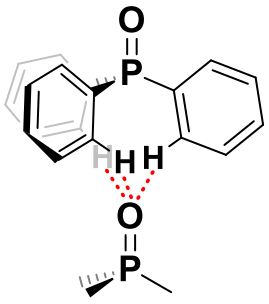
BP86-D3/def2-SVP



(C_3 propeller geometry)

P	-0.00036400	-0.00164400	0.93208700
C	0.02486500	4.34019900	-0.72734700
C	-0.49260500	3.31588100	-1.54102800
H	-0.88021200	3.55061300	-2.54521600
C	-0.52843600	1.99199800	-1.06944700
H	-0.95952600	1.19632600	-1.69843100
C	-0.03437300	1.69092400	0.21746900
C	0.46950900	2.72182500	1.03858600
H	0.81762400	2.46932000	2.05321500
C	0.50023600	4.04332500	0.56338300
H	0.89180200	4.84804200	1.20592700
O	0.00058600	-0.00225700	2.45282900
C	-3.77447800	-2.14762100	-0.72798000

C	-2.62704900	-2.08876700	-1.53977300
H	-2.63571500	-2.54521800	-2.54242700
C	-1.46224500	-1.45830500	-1.06836800
H	-0.55652200	-1.43743900	-1.69584000
C	-1.44946300	-0.87634900	0.21703700
C	-2.59606600	-0.94996300	1.03613300
H	-2.55274300	-0.51883200	2.04939200
C	-3.75651100	-1.58265000	0.56067200
H	-4.65074000	-1.64128100	1.20153200
C	3.75125200	-2.18826400	-0.72632600
C	3.12367000	-1.22669800	-1.53912700
H	3.52325900	-1.00505800	-2.54159400
C	1.99279700	-0.53658800	-1.06875600
H	1.52027600	0.23594100	-1.69684100
C	1.48279900	-0.81722000	0.21668100
C	2.12265400	-1.77068700	1.03668400
H	1.72746500	-1.94936700	2.04975700
C	3.25335300	-2.45583200	0.56232000
H	3.75341700	-3.19876800	1.20400200
H	0.04802700	5.37747600	-1.09790400
H	-4.68478900	-2.64547100	-1.09848600
H	4.63969100	-2.72481200	-1.09590200
Sum of electronic and zero-point Energies=			-1110.682460
Sum of electronic and thermal Energies=			-1110.665273
Sum of electronic and thermal Enthalpies=			-1110.664329
Sum of electronic and thermal Free Energies=			-1110.729451



(C_{3v} geometry)

P	1.94207000	-0.00005700	-0.69319700
C	-0.45617700	-3.81850200	-1.85653900
C	-0.95237400	-3.00982400	-0.81723700

H	-1.87805600	-3.29640200	-0.29094000
C	-0.27067200	-1.84191000	-0.43199200
H	-0.69149200	-1.22230200	0.37547500
C	0.92256700	-1.48365600	-1.09321400
C	1.42621500	-2.29674600	-2.13060000
H	2.36840700	-1.99911600	-2.61870400
C	0.73454000	-3.45925400	-2.51265800
H	1.13133200	-4.09084400	-3.32366200
O	3.24368500	-0.00010700	-1.48718900
C	-0.45585700	3.81860300	-1.85649700
C	-0.95216000	3.00991400	-0.81725400
H	-1.87783800	3.29654600	-0.29098100
C	-0.27058100	1.84191300	-0.43205200
H	-0.69147700	1.22229300	0.37537000
C	0.92267500	1.48361500	-1.09321900
C	1.42642900	2.29671400	-2.13054700
H	2.36862400	1.99903900	-2.61861600
C	0.73485800	3.45929000	-2.51258500
H	1.13173800	4.09089200	-3.32353600
C	2.94936200	-0.00006800	3.84605000
C	1.59318700	0.00002100	3.47222400
H	0.80561700	0.00008600	4.24254100
C	1.22586100	0.00002300	2.11544600
H	0.15354700	0.00009500	1.86541600
C	2.23245200	-0.00005900	1.12310600
C	3.59354300	-0.00014400	1.49818300
H	4.35718800	-0.00020500	0.70365300
C	3.94911500	-0.00015000	2.85744700
H	5.01282000	-0.00021700	3.14500800
O	-2.05631300	0.00001500	1.56330700
P	-3.41750900	0.00006100	0.87054800
C	-4.43518400	1.45857400	1.31425700
H	-4.54747400	1.48972200	2.41638000
H	-3.89804700	2.37235300	0.98984300
H	-5.43497600	1.42798700	0.83573500
C	-4.43530500	-1.45834200	1.31434000
H	-4.54759000	-1.48942200	2.41646600
H	-5.43509700	-1.42769400	0.83582300
H	-3.89824700	-2.37218300	0.98996900

C	-3.33703000	-0.00000600	-0.95911500
H	-4.35207300	-0.00000100	-1.40547100
H	-2.77762800	0.89691100	-1.29276900
H	-2.77766400	-0.89697300	-1.29269900
H	-0.99482100	-4.73372100	-2.15063000
H	-0.99441400	4.73388100	-2.15056300
H	3.22743100	-0.00007200	4.91242500

Sum of electronic and zero-point Energies= -1646.726392

Sum of electronic and thermal Energies= -1646.699791

Sum of electronic and thermal Enthalpies= -1646.698847

Sum of electronic and thermal Free Energies= -1646.785271

O	-0.00161900	0.00201700	1.70323800
P	-0.00037300	0.00026500	0.18926200
C	1.08255600	1.28295700	-0.56579400
H	0.74603500	2.27867700	-0.21321700
H	2.11952100	1.11993100	-0.20914600
H	1.06107100	1.25343200	-1.67447200
C	-1.65233000	0.29425700	-0.56705500
H	-2.02991200	1.27492800	-0.21388100
H	-1.61554400	0.28659800	-1.67567000
H	-2.34614500	-0.49408500	-0.21191600
C	0.57156000	-1.57928200	-0.56343600
H	0.55674500	-1.54713100	-1.67217400
H	1.60254400	-1.78330300	-0.21067500
H	-0.08648800	-2.39674700	-0.20598000

Sum of electronic and zero-point Energies= -536.021410

Sum of electronic and thermal Energies= -536.013609

Sum of electronic and thermal Enthalpies= -536.012665

Sum of electronic and thermal Free Energies= -536.052230

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