Content

1 Experimental Section

General procedures. All manipulations were performed under an atmosphere of dry argon using standard Schlenk techniques or in an MBraun glovebox. Solvents (dichloromethane, *n*-pentane, and toluene) were dried and degassed by means of an MBraun SPS-800 solvent purification system. Deuterated solvent for NMR spectroscopy ($CDCl_3$) as well as *o*-dichlorobenzene were dried and degassed at reflux over CaH_2 and freshly distilled prior to use. Boron tribromide, 1-bromo-2,4,6-trimethylbenzene, magnesium turnings and solutions of *n*-butyllithium (1.6 M in hexane and 2.5 M in hexane, respectively) were commercially purchased and used as received. Chlorotrimethylsilane was distilled prior to use and Cu(I)Cl was purified according to literature procedure.[1] MesCu,[2] $MesBBr_2$,[3] **1**,[4] **2**,[4] and **4**[4] were prepared according to methods described in the literature. ^{1}H- and ^{31}P-NMR spectra were recorded on a Varian VNMRS-500 MHz-spectrometer at 20°C. Further NMR spectra were recorded at 25 °C on a Bruker AVANCE II-400 spectrometer or on a Bruker Advance III HD spectrometer operating at 400 MHz. Chemical shifts were referenced to residual protic impurities in the solvent (^{1}H) or the deuterio solvent itself (^{13}C) and reported relative to external $SiMe_4$ (^{1}H, ^{13}C) or $BF_3{\cdot}OEt_2$ (^{11}B) standards. Mass spectra were obtained with the use of a Finnigan MAT95 spectrometer employing electron ionisation (EI) using a 70 eV electron impact ionisation source. Elemental analysis was performed with a HEKAtech Euro EA CHNS elemental analyzer. Samples were prepared in a Sn cup and analyzed with added V_2O_5 to ensure complete combustion. UV–vis spectra were obtained using a Shimadzu UV mini1240 spectrophotometer. Melting points (uncorrected) were obtained using a SMP3 melting point apparatus by Stuart in 0.5 mm (o.d.) glass capillaries, which were sealed under argon. X-ray crystallographic data were collected on a Bruker SMART APEX CCD detector on a D8 goniometer equipped with an Oxford Cryostream 700 temperature controller at 100(2) K using graphite monochromated Mo-K_α radiation (λ = 0.71073 Å). An absorption correction was carried out semi-empirically using SADABS[5] (min./max. transmissions = 0.6725/0.7461 (**3**). The structure was solved with Olex2[6] using Direct Methods (ShelXS[7a]) and refined with the ShelXL[7b] refinement package by full-matrix least squares on F^2. All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were included isotropically and treated as riding. Cyclic voltammetric, chronoamperometric and dual electrode measurements were carried out in an MBraun acrylic glovebox GB2202-C-VAC under inert argon atmosphere. All samples were measured in dichloromethane, which was dried over CaH_2, distilled and stored over molecular sieves (3 Å) under argon atmosphere. Tetrabutylammonium hexafluorophosphate ($[NBu_4][PF_6]$) served as supporting electrolyte with a concentration of 0.1 mol L^{-1}.

The sample concentration during the measurements was set to 0.1 mmol L^{-1}. For cyclic voltammetric measurements the setup consisted of a three-electrode cell with a platinum disk as working electrode, a silver spiral as counter electrode and a silver pseudo reference electrode. For Differential Pulse Voltammetry (DPV) the same set up was used. The plotted DPV was measured with a pulse amplitude of 50 mV and 10 mV increment. The pulses were maintained for 50 ms and sampled 3 ms pre- and post-pulse (pulse period 100 ms). Dual electrode voltammetry experiments as well as chronoamperometric measurements were carried out with a Modulated Speed Rotator ring-disk system from Pine Research Instrumentation including a mirror polished glassy carbon 5.0 mm OD disk insert and a 6.5 (ID)/7.5 (OD) mm platinum ring. The sweep rate was always 100 mV s^{-1}, the disk electrode potential was driven from 0 to 900 resp. 1000 mV and the ring electrode potential held at 0 mV. While the potential was driven on the WaveDriver 20 Bipotentiostat from Pine Research Instrumentation, electrochemical data were recorded via AfterMath (Ver. 1.2.5966; Pine Instruments). The half wave potentials of the redox processes, which were referenced using decamethyl ferrocene, and current data of the dual electrode measurements were evaluated with OriginPro (Ver. 8.6.0; OriginLab Corporation). To calculate the rate constant *k* of the consecutive reaction the diffusion coefficient $D = 1.9(2) \cdot 10^{-9}$ m^2 s^{-1} was determined by chronoamperometric measurements at 700 mV for 30 s and evaluation via Cottrell-Plot.[8] Furthermore, the kinematic viscosity ν was calculated on the supposition that the volume of the solvent and its dynamic viscosity does not change with the addition of supporting electrolyte.

Synthesis of 3.

Route A:

To a solution of **1** (181.1 mg, 0.50 mmol) in toluene (2.5 mL) was added a solution of *n*-butyllithium (2.5 M, 1.05 mmol, 0.42 mL) dropwise at 0 °C. The mixture was stirred for 12 h resulting in the formation of the dilithiated species **2** suspended in toluene. After cooling to −78 °C, $MesBBr_2$ (144.9 mg, 0.50 mmol) was added dropwise. The reaction mixture was slowly warmed to room temperature and stirred overnight. After filtration and extraction of the solid residue twice with toluene (5 mL), the combined organic phases were evaporated to dryness. The product was purified by recrystallization from *n*-pentane/dichloromethane (5:1) at −40 °C to yield **3** as orange crystals (m.p. 191 °C). Yield: 68.7 mg (0.35 mmol, 28 %). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 6.80 (br s, 2H; Mes-C-*H*), 4.42 (m_c, 4H, Cp-α-C*H*), 4.39 (m_c, 4H, Cp-β-C*H*), 2.50 (t, $^5J_{PH}$ = 1.8 Hz, 6H; Mes-*o*-CH_3), 2.27 (s, 3H; Mes-*p*-CH_3), 0.93 ppm (m_c, 18H, *t*Bu-CH_3); ^{11}B{^{1}H} NMR (128 MHz, $CDCl_3$): δ = 77.5 ppm (s); ^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ = 140.0 (br s, Mes-*C*-B), 136.3 (s, Mes-*C*–*p*-CH_3), 135.6 (t, $^3J_{PC}$

= 6 Hz, Mes-*C*–*o*-CH_3), 128.0 (s, Mes-*C*H), 78.6 (t, $^2J_{PC}$ = 7 Hz, Cp-α-*C*), 72.8 (t, $^3J_{PC}$ = 3 Hz, Cp-β-*C*), 69.8 (t, $^1J_{PC}$ = 10 Hz, Cp-*ipso*-*C*), 35.0 (s, *t*-Bu-*C*), 30.4 (t, $^2J_{PC}$ = 5 Hz, *t*-Bu-CH_3), 25.2 (t, $^4J_{PC}$ = 6 Hz, Mes–*o*-CH_3), 21.1 ppm (s, Mes-*p*-CH_3); ^{31}P NMR (202 MHz, $CDCl_3$): δ = 9.9 ppm (s); MS (EI, 70 eV): *m/z* (%) = 490.2 (M^+, 47), 433.1 ([ferrocenediyl(P_2*t*Bu)BMes]$^+$, 62), 305.1 ([ferrocenediyl(PH_2P*t*Bu)]$^+$, 100) 249.0 ([ferrocenediyl(P_2H_3)]$^+$, 46), 186.1 ([ferrocene]$^+$, 36); HRMS: calcd for $C_{27}H_{37}BFeP_2$: 490.1807, found: 490.1800; elem. anal. calcd (%) for $C_{27}H_{37}BFeP_2$: C 66.16, H 7.61, found: C 66.08, H 7.55; UV–vis (CH_2Cl_2): $\lambda_{abs,max}$ = 347 nm (ε = 33306 L mol^{-1} cm^{-1}); UV–vis (*n*-pentane): $\lambda_{abs,max}$ = 344 nm; UV–vis (toluene): $\lambda_{abs,max}$ = 346 nm; UV–vis (*o*-DCB): $\lambda_{abs,max}$ = 347 nm.

Route B:

To a solution of **4** (260.8 mg, 0.50 mmol) in dichloromethane (2.5 mL) was added $MesBBr_2$ (144.9 mg, 0.50 mmol) dropwise at −78 °C. The mixture was slowly warmed to room temperature and stirred overnight. All volatiles were removed *in vacuo* and the crude product was purified by recrystallization from *n*-pentane/dichloromethane (5:1) at −40 °C to yield **3** as orange crystals. Yield: 172.1 mg (0.35 mmol, 70 %).

X-ray crystallographic analysis of 3. Suitable colorless single crystals of **3** ($C_{27}H_{37}BFeP_2$, M = 490.17 g mol^{-1}) were obtained from a concentrated *n*-hexane solution by cooling to −40 °C. Crystal size 0.12 x 0.11 x 0.11 mm, monoclinic, $P2_1/c$, a = 9.9177(4), b = 11.5650(5), c = 22.0296(9) Å, V = 2520.82(18) Å^3, Z = 4, ρ_{calc} = 1.292 Mg · m^{-3}, 3.7° ≤ 2θ ≤ 61.86°, collected (independent) reflections = 37814 (7498), R_{int} = 0.0364, μ = 0.738 mm^{-1}, 362 refined parameters, 0 restraints, $R1$ (I > 2σ(I)) = 0.0349, $R1$ (all data) = 0.0426, $wR2$ (I > 2σ(I)) = 0.1106, $wR2$ (all data) = 0.1217, residual electron density = 0.56/−0.39 e · Å^{-3}. CCDC-1574232 contains the supplementary crystallographic data for the structure of **3**. This data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

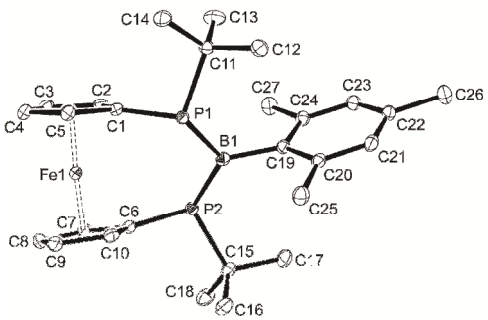


Figure S1. Molecular structure of **3** in the solid state with thermal ellipsoids set at 50 % probability (hydrogen atoms omitted for clarity).

NMR spectra

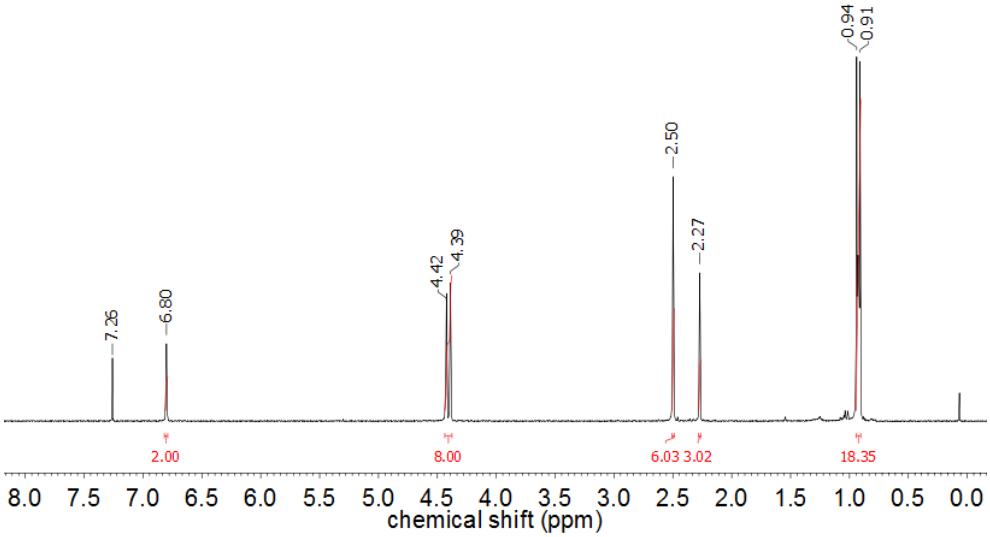


Figure S2. ^{1}H NMR spectrum of **3** (500 MHz, in $CDCl_3$).

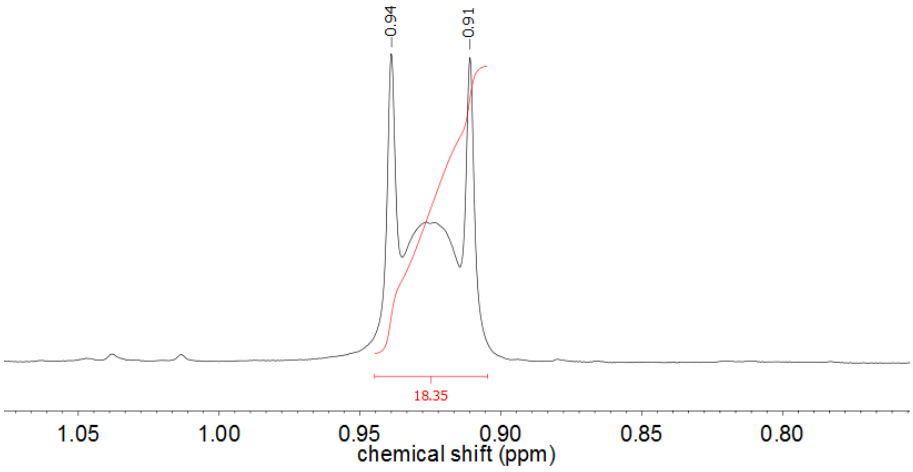


Figure S3. ^{1}H NMR spectrum of **3** (detail of *t*Bu-signal) (500 MHz, in $CDCl_3$).

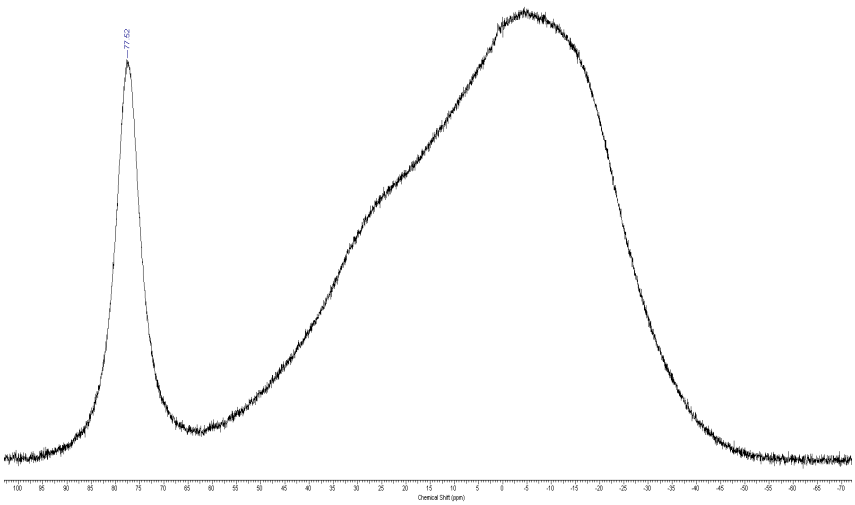


Figure S4. ^{11}B{^{1}H} NMR spectrum of **3** (128 MHz, in $CDCl_3$).

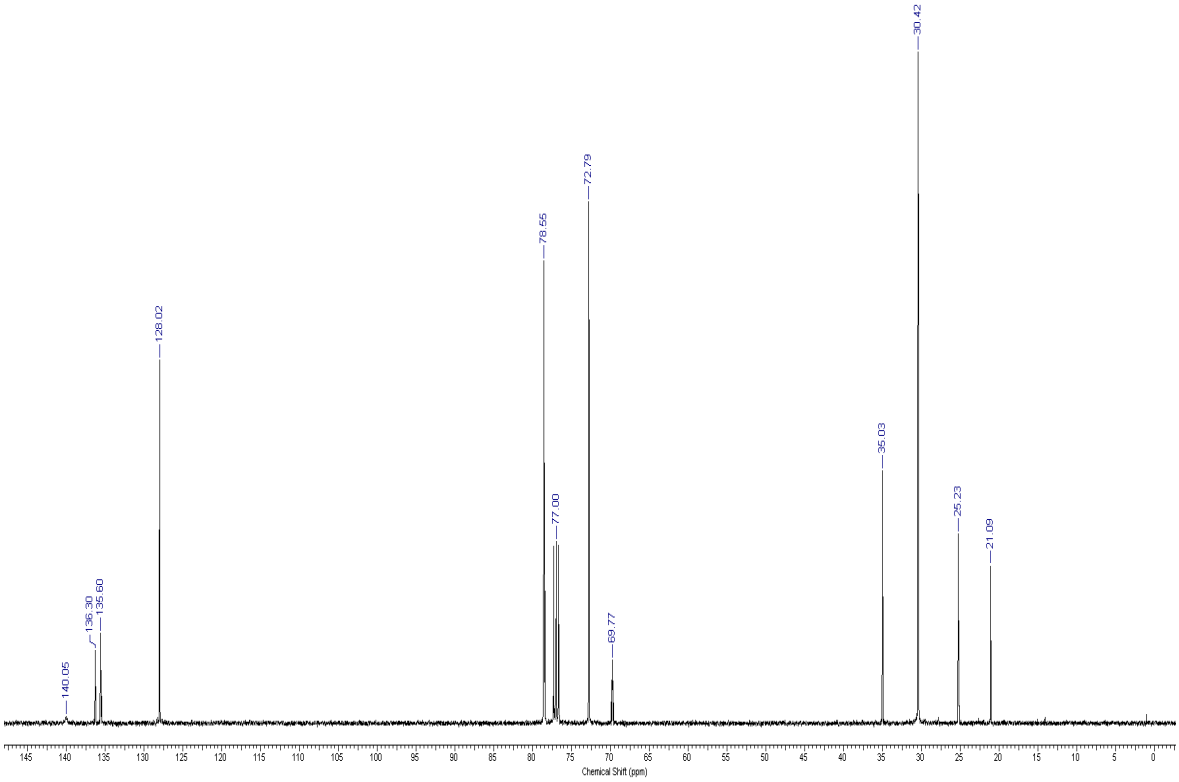


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **3** (101 MHz, in $CDCl_3$).

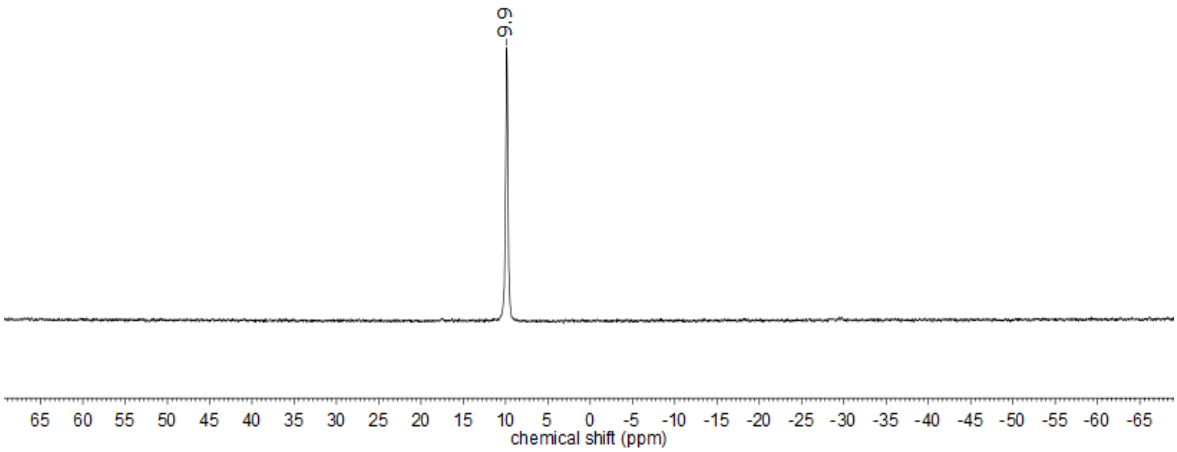


Figure S6. ^{31}P NMR spectrum of **3** (202 MHz, in $CDCl_3$).

UV–vis spectroscopy

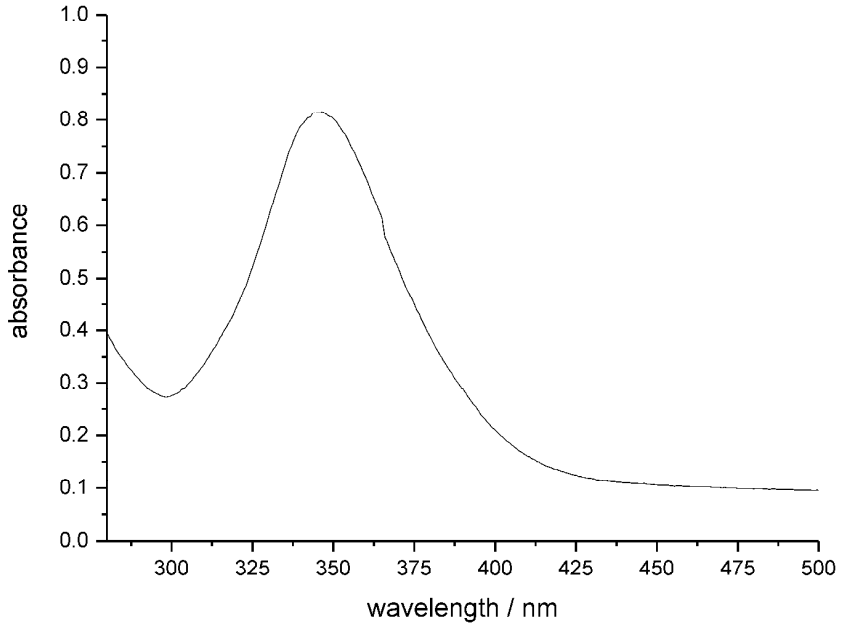


Figure S7. UV–vis spectrum of **3** (in CH_2Cl_2).

Mass spectrometry

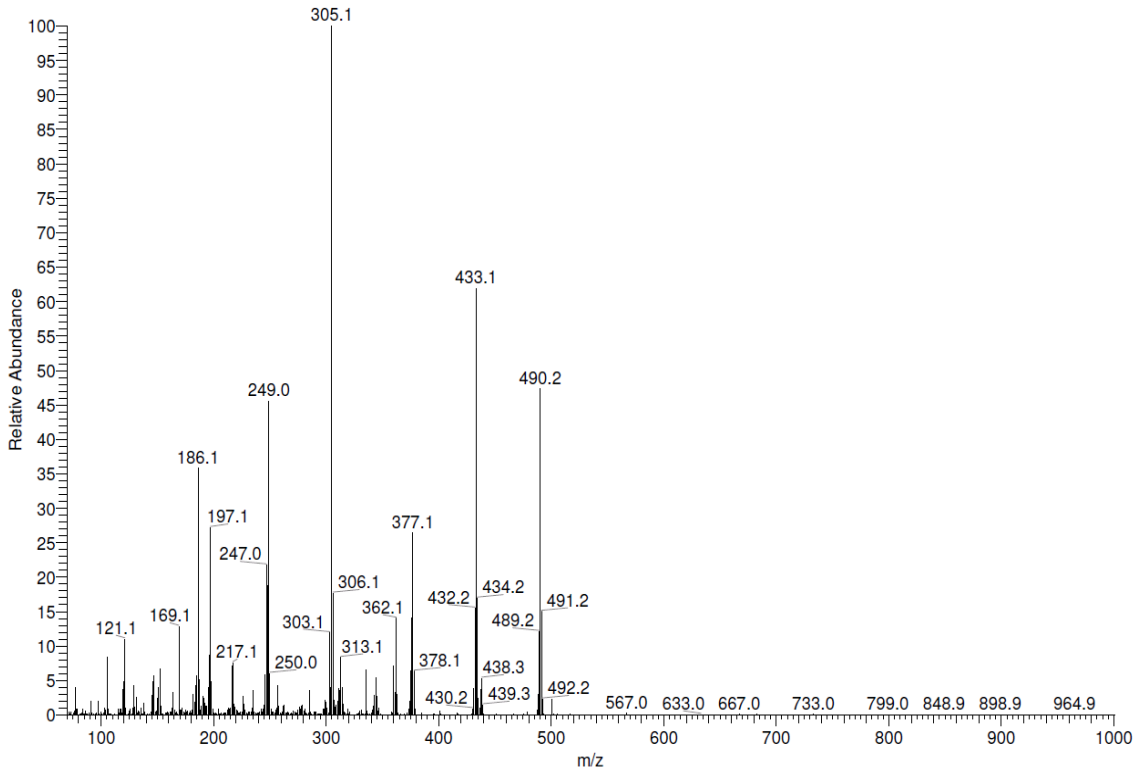


Figure S8. EI mass spectrum of **3**.

Electrochemical measurements

Our cyclic voltammetric studies of **3** reveal two irreversible electrochemical responses for the oxidation in dichloromethane (scan rate: 250 mV s^{-1}; with peak potentials E_p = +0.29(1) V and +0.82(1) V vs. Fc/Fc^+; Figure S9) before reaching a broad irreversible downstream process at around +1 V (vs. Fc/Fc^+) which indicates several similar follow up oxidations (black line; Figure S9). Differential pulse voltammetry measurements (Figure S12), which are particular useful to determine overlapping consecutive electron transfers, unveiled three oxidations events subsequent to the antecedent. Reversing the potential sweep after the first oxidation process, which is assigned to oxidation of the ferrocene backbone, leads to a "more reversible" redox response for this particular process (red line; Figure S9). With increasing scan rate up to 1 V s^{-1}, leaving the system less time to react, the oxidation behavior finally turns into quasi reversible (blue line; Figure S9). This behavior demonstrates the presence of a consecutive reaction after oxidation of the ferrocene backbone. It is known from literature that monocations of substituted ferrocenes can exhibit less stability.[9] Increased scan rates may overcome the decomposition of the corresponding ferrocenium species. Recently, a similar phenomenon was observed for PPP congeners of **3**, i.e. compounds **VI** (cf. Scheme 1 in the main article).[10]

To get deeper insight in the electron transfer mechanism of the follow up reaction, we extended our investigations using dual electrode methods. The established rotating ring-disk electrode (RRDE) system produces a flux of analyte towards the central disk electrode. Radial components of the stream transport the primary oxidation product, generated at the disk, to the outer ring electrode. In transit, it may undergo follow up reactions whose products can be electrochemically analyzed at the ring. Due to diffusion effects, even without consecutive reactions only a small proportion of generated intermediates reach the ring electrode. The collection efficiency depends on the electrode geometry and is defined as

$$N = \frac{nI_R}{qI_D}$$

with n resp. q electrons, ring current I_R and disk current I_D.

For non-reversible oxidations the collection efficiency N_k shows dependencies from both the electrode geometry and the rotation rate ω. Ring and disk current increase with increasing rotational speed (see Figure S10). From the deviation of the measured N_k values and the undisturbed N value (taken from reversible oxidized ferrocene) it was possible to calculate the rate constant k of the consecutive reaction.

According to Albery and Hitchman[11] a simple correlation to k is obtained using following equation:

$$\frac{1}{N_k} = \frac{I_D}{I_R} = \frac{1}{N} + \frac{1{,}28}{N}\left(\frac{\upsilon}{D}\right)^{1/3}\frac{k}{\omega}$$

with the kinematic viscosity ν and the diffusion coefficient D.

From the slope of the linear plot ($1/N_k$ over $1/\omega$; see Figure S11) the rate constant k was assigned to 3.2(4) s^{-1}, corresponding to an average lifetime τ of the oxidized intermediate of 0.31(4) s.

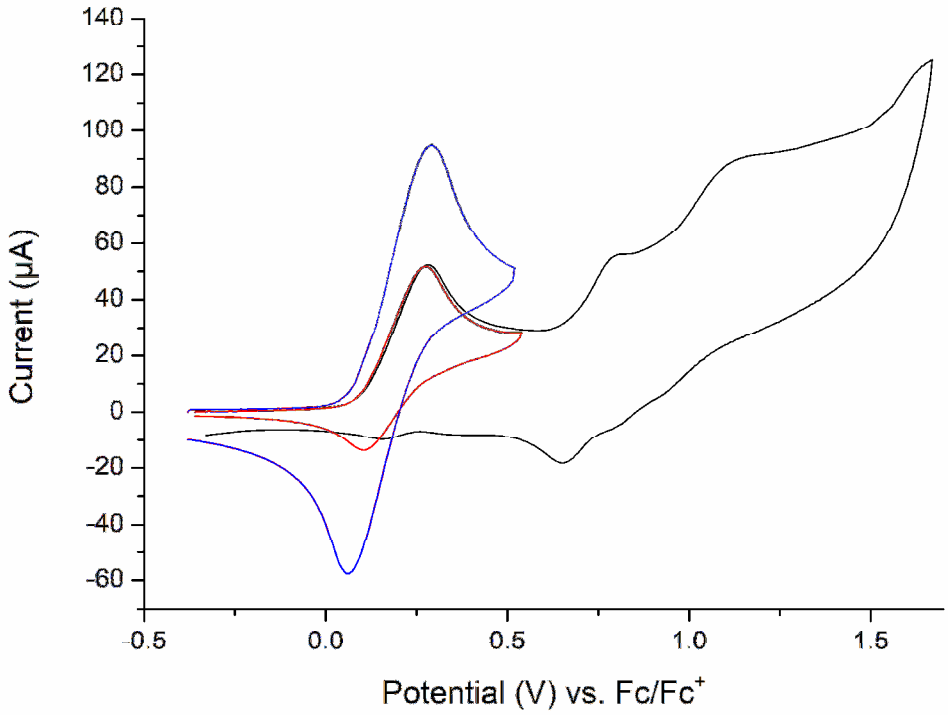


Figure S9. Overlay of cyclic voltammetric measurements of **3**. Black: Overview at 250 mV s^{-1}. Red: "More reversible" oxidation behavior at 250 mV s^{-1} returning after the first oxidation. Blue: Quasi reversible oxidation behavior at high sweep rates (1000 mV s^{-1}).

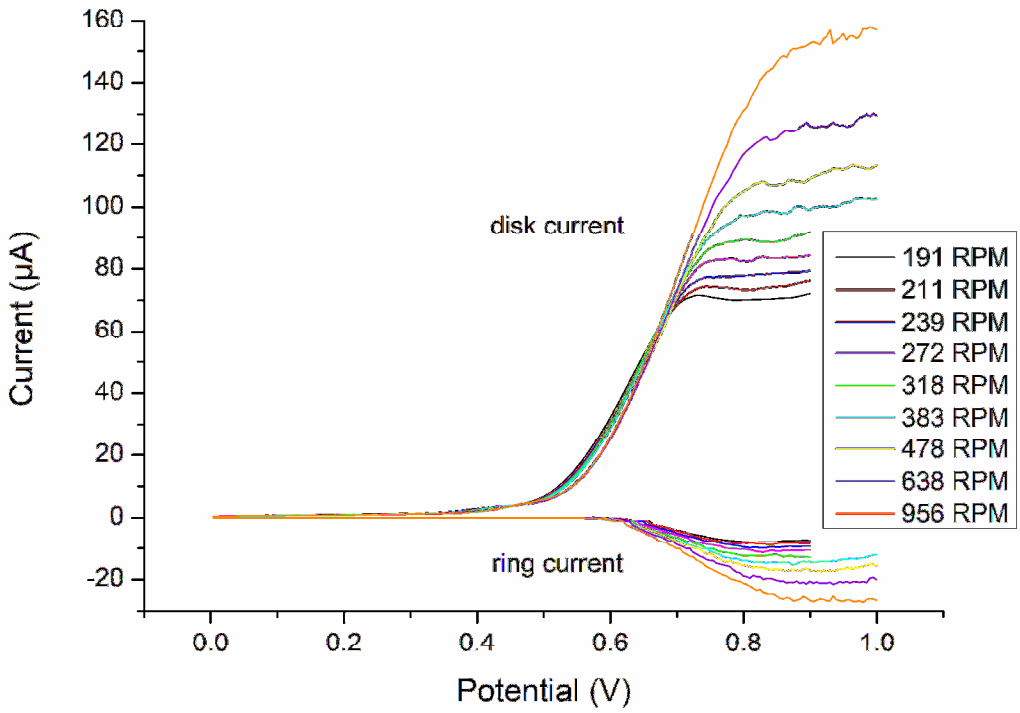


Figure S10. Disk (positive values) and ring (negative values) current in dual electrode experiments at different rotation speeds of the electrodes.

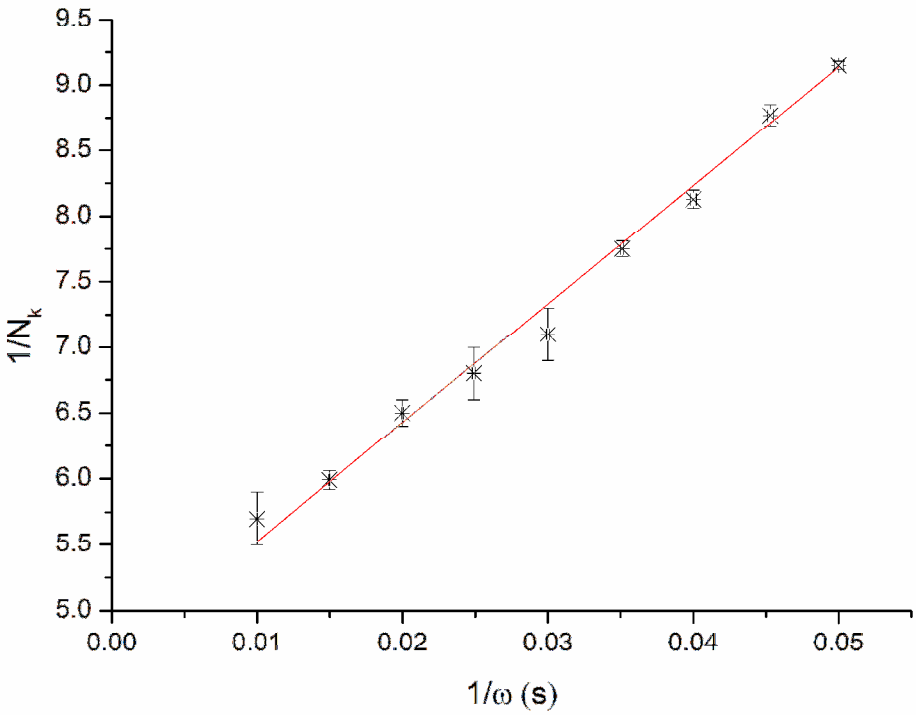


Figure S11. Albery-Hitchman-Plot. The linear fit exhibits a slope of 90(2) s^{-1}.

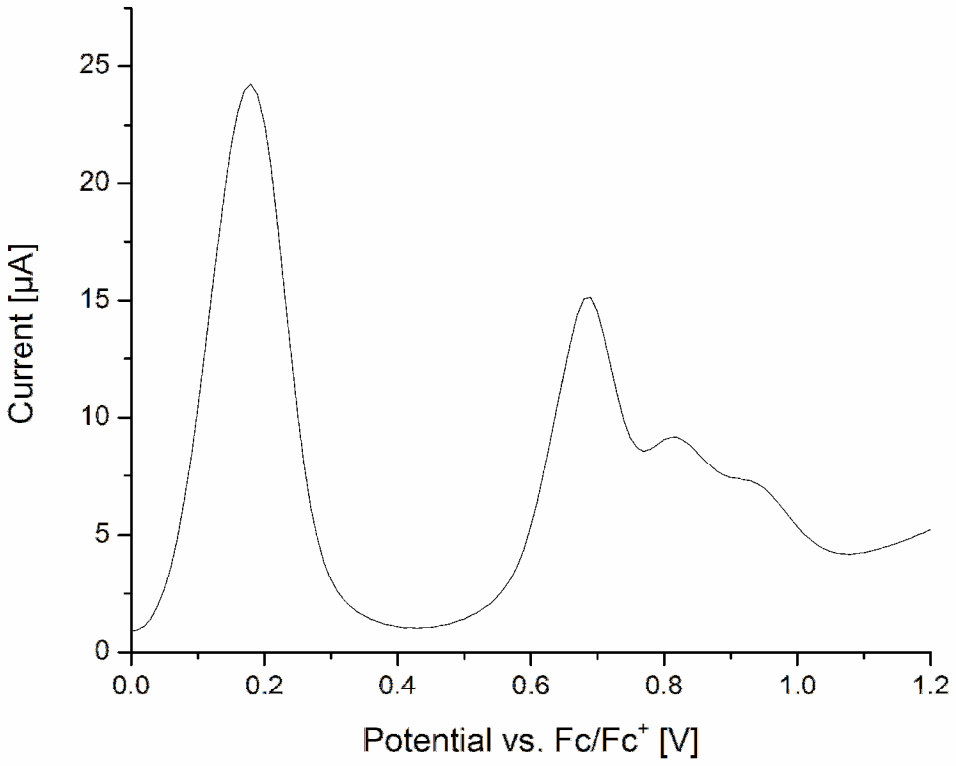


Figure S12. Differential Pulse Voltammetry of **3**.

2 Computational Information

All calculations were carried out with the Gaussian 09 program package.[12] Full geometry optimization calculations were performed. Harmonic vibrational frequencies were calculated at that level, which was used for the optimization to establish the nature of the stationary points obtained, as characterized by none or a single negative eigenvalue of the Hessian for minima and transition structures, respectively. It should be noted in some cases calculation at different level of theory were also performed (Figure S14, Table S4), which gave similar results to the results at B3LYP/6-311+G** level of theory, which was earlier used for ferrocene containing systems.[4,10] For the radical cations, unrestricted B3LYP/6-311+G** calculations were carried out. The <S2> values (see Table S3) of these systems were close to the theoretical 0.75, which suggests that they do not have significant multireference character. We also carried out single point calculations using the BPE0 method, which was successfully applied for ferrocene containing radical systems[13] and gave similar results to our calculations at B3LYP/6-311+G** level of theory. Bond orders and bond critical points and their properties were calculated with Multiwfn program.[14] For the visualization of the molecular structures and the molecular orbitals the MOLDEN,[15] Gaussview,[16] and VMD program[17] were used.

Bonding situation of 3

To understand the bonding situation of **3**, different reference compounds (Figure S13) were also calculated and compared the properties of the B-P bond of them (Table S1). (In case of **D** and **E** the related *cis* isomers (**D_{cis}** and **E_{cis}**) were also computed and although the energy difference between them are small (E_D-E_{Dcis}=-0.5 kcal mol^{-1} E_E-E_{Ecis}=1.0 kcal mol^{-1}) only the *trans* isomers were in more details investigated, since the observed **3** exhibits *trans* configuration.)

While the calculated two B-P bond lengths in **3** are very close to each other (at B3LYP/6-311+G** level of theory) – similar to the parent $HB(PH_2)_2$ and **D** – in case **B**, **C** and **E** compounds the two B-P bonds differ significantly. Both phosphorus atoms in **3** exhibit high pyramidal character, in good agreement with the donor-acceptor interaction between the phosphorus lone pairs and the boron center, which is 37.3 and 37.6 kcal mol^{-1} according to our second order perturbation analysis of the Fock matrix in NBO basis. For the better comparison of the interactions between the different compounds it is worth to sum up the interaction energies between the lone pairs of phosphorus and boron center ($\sum E_{E-P}$). As we can see in Table S1, **3** has one of the largest $\sum E_{E-P}$ value among the investigated systems. The increased $\sum E_{E-P}$ value of **3** can be explained by the ferrocene backbone which behaves as a spacer between the two phosphorus atoms and increases the bond angles around the phosphorus. Similar statement can be established in case of the six-membered ring containing **E** compound.

The NBO calculation and the planar phosphorus atoms indicate a strong interaction between the phosphorus and the boron center, thus suggesting double bond character. Established measures for bond orders (see in Table S1, Mayer, Wiberg) are smaller for **3** than for the other reference compounds. The single bond character was also verified by the small ellipticity of the electron density in the B-P bond critical point.

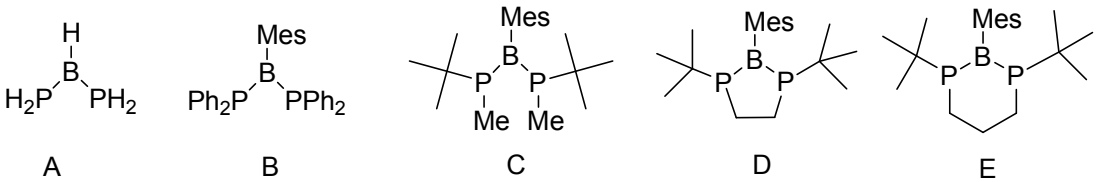


Figure S13. Reference compounds for the comparison of the bonding situation of **3**.

Table S1. Different properties of the B-P bond in case of **3** and **A-E** compounds.

		3	A	B	C	D	E
calculated P-B bond length	B-P(1)	1.904	1.892	1.913	1.887	1.902	1.875
	B-P(2)	1.904	1.892	1.903	1.945	1.902	1.908
sum of bondangles around the P center	P(1)	332.2	301.7	333.6	336.2	323.3	336.4
	P(2)	332.1	301.7	324.1	319.9	323.0	326.0
P->B donation energy from the NBO	$E_{B-P(1)}$	37.6	15.8	37.2	49.5	27.8	47.6
	$E_{B-P(2)}$	37.3	15.8	26.6	12.9	27.3	27.9
	$\sum E_{E-P}$	74.9	31.6	63.8	62.4	55.1	75.5
Mayer bond order	B-P(1)	1.53	1.25	1.84	2.26	2.24	2.31
	B-P(2)	1.54	1.25	1.72	1.85	2.21	2.92
Wiberg bond order	B-P(1)	1.18	1.47	1.18	1.30	1.20	1.27
	B-P(2)	1.18	1.47	1.15	1.13	1.20	1.17
electrondensity in the B-P bondcritical point	B-P(1)	0.140	0.146	0.139	0.142	0.142	0.144
	B-P(2)	0.140	0.146	0.140	0.135	0.142	0.141
ellipticity of the electrondensity in the B-P bondcritical point	B-P(1)	0.05	0.01	0.06	0.05	0.05	0.03
	B-P(2)	0.05	0.01	0.03	0.06	0.05	0.03

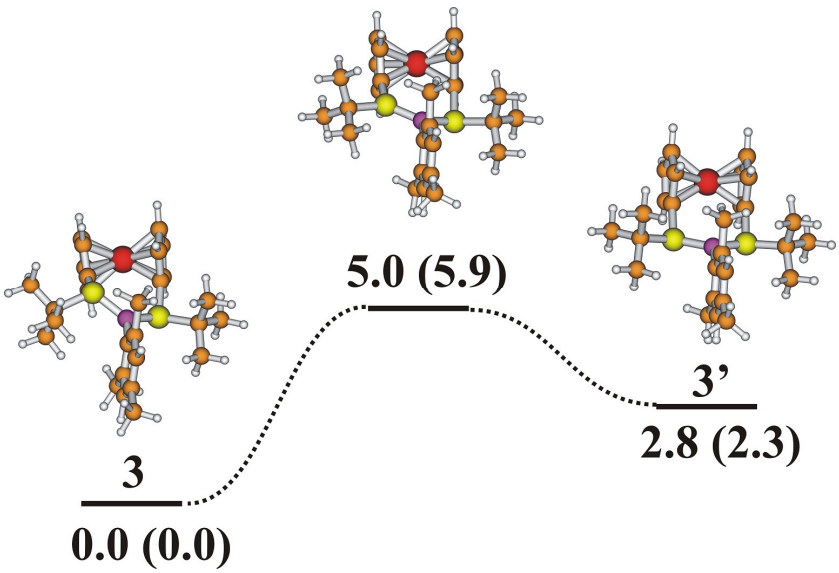


Figure S14. The inversion barrier (ΔE) of **3** and the less stable **3'** isomer, which was not observed, at B3LYP/6-311+G** level of theory (at ωB97X-D/6-311+G** level of theory in brackets) and in kcal mol^{-1} unit.

TD-DFT calculations

TD-DFT calculations at B3LYP/6-311+G** level of theory suggest four close lying transitions in case of **3**, which involve the (admixture of the) excitations from the HOMO-X (X=0,1,2,3) to the LUMO (Table S2). The charge density difference maps (Table S2) show clearly that the excitations at 352, 348 and 332 nm have significant charge transfer character. They can be mainly regarded as a transition from the iron towards the PBP unit. We have also computed the related *cis* isomer (**3**$_{cis}$, **Table 3**). In the near UV region three transitions (intensity >0.005) were found. While the excitation at 364 nm exhibits no charge transfer character which is contradicted with the case of the *trans* isomer (the excitation of **3** at 352 nm), the two other excitations show the same charge transfer character as the *trans* isomer. The reason of this phenomena is the different shape of the occupied orbitals in the two isomers (Figure S15). While in both cases the LUMO are localized at the PBP unit, in case of **3** both the iron and the PBP unit have significant contribution to the HOMO, HOMO-1, HOMO-2, in case of **3**$_{cis}$ the HOMO is localized mainly at the phosphorus, while to the HOMO-1 and HOMO-2 the iron center has contribution. Thus the excitation at 364 nm in case of **3**$_{cis}$ (Table S3) shows no charge transfer character since it can be mainly regarded a HOMO-LUMO transition (transition from the phosphorus lone pairs to the PBP unit).

Table S2. TD-DFT results. The charge density difference map show the regions where the electron density increased (blue) and decreased (red) after electron excitation.

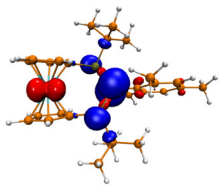
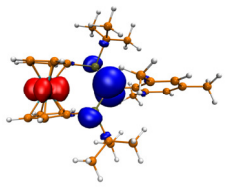
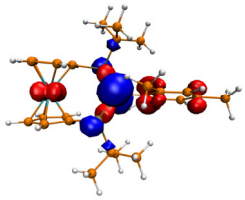
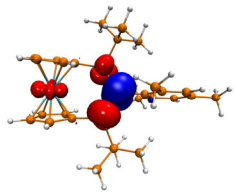
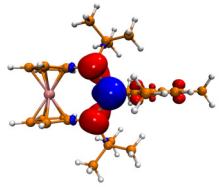
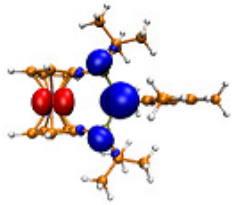
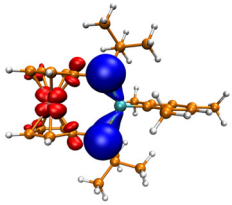
λ_{abs} (nm)		Intensity	Transition	Coefficient	Charge density difference map
Exp.	Calc.				
347	352	0.0215	HOMO-3→LUMO	0.10	
			HOMO-1→LUMO	0.69	
	348	0.0286	HOMO-2→LUMO	0.41	
			HOMO →LUMO	0.57	
	332	0.0177	HOMO-3→LUMO	0.69	
			HOMO-1→LUMO	-0.11	
	329	0.1201	HOMO-2→LUMO	0.57	
			HOMO-1→LUMO	-0.40	

Table S3. TD-DFT results. The charge density difference map show the regions where the electron density increased (blue) and decreased (red) after electron excitation.

λ_{abs} (nm)		Intensity	Transition	Coefficient	Charge density difference map
Exp.	Calc.				
347	364	0.0753	HOMO-3→LUMO	-0.12	
			HOMO→LUMO	0.69	
	338	0.0052	HOMO-2→LUMO	0.56	
			HOMO-1→LUMO	0.42	
	320	0.0108	HOMO→LUMO+2	0.69	

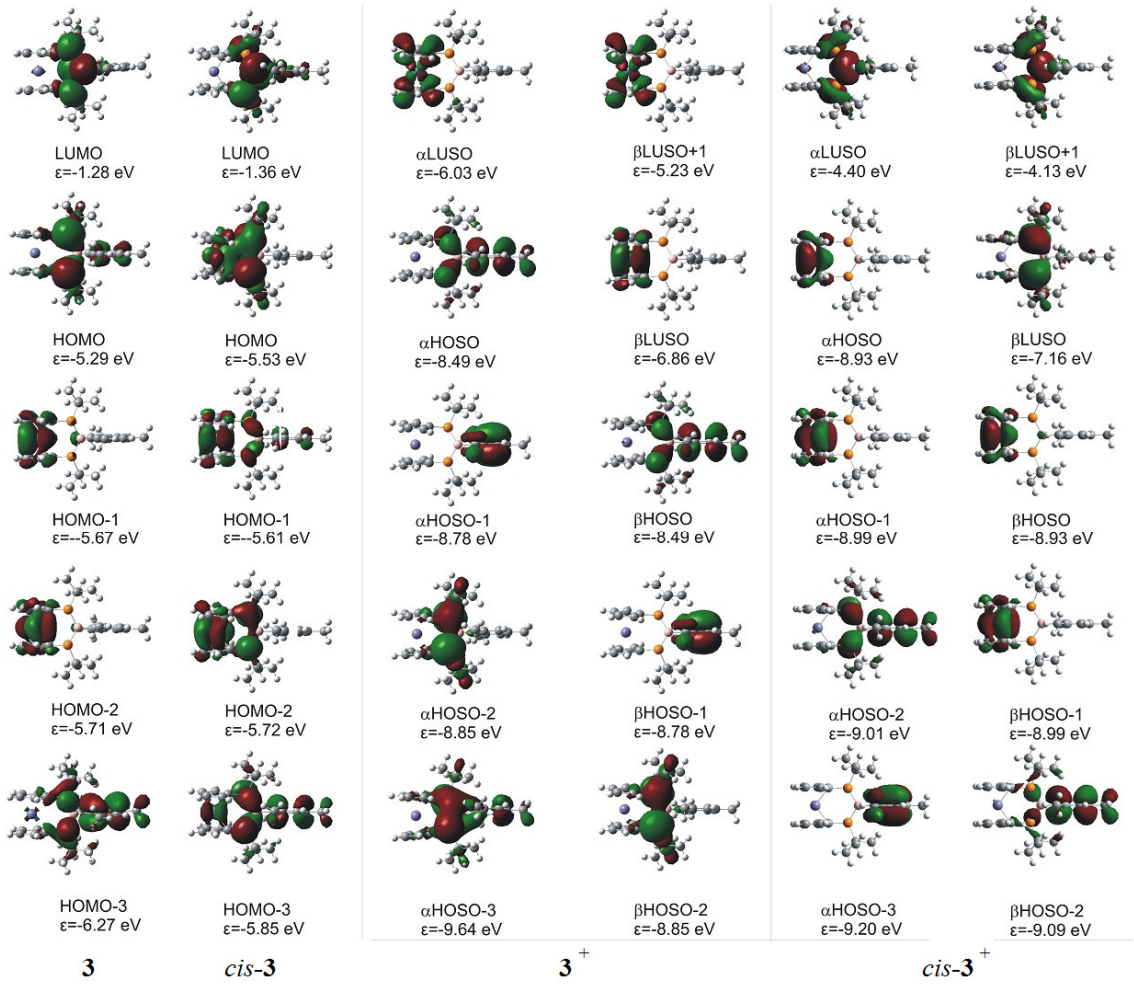
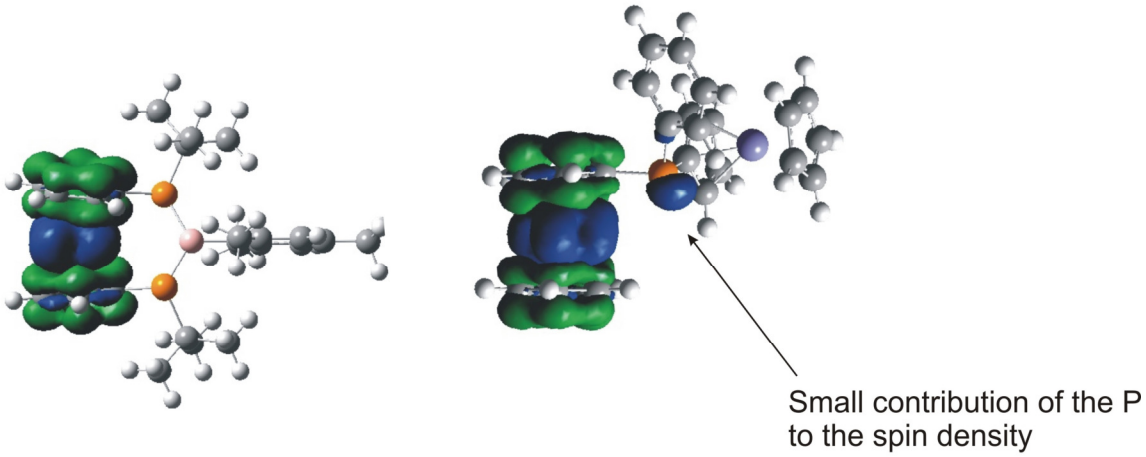


Figure S15. Selected Kohn-Sham orbitals at B3LYP/6-311+G** level of theory of **3**, **3**$^{+}$ and the related cis isomers of (**3**$_{cis}$, **3**$_{cis}^{+}$).

Table S4. The <S2> values of **3**$^{+}$ and **3**$_{cis}^{+}$ at different level of theory.

level of theory	**3**$^{+}$	**3**$_{cis}^{+}$
B3LYP/6-311+G**	0.787	0.775
B3LYP/6-31G*//B3LYP/6-311+G**	0.783	0.774
B3LYP/cc-pVTZ//B3LYP/6-311+G**	0.787	0,776
M06-2X/6-311+G**//B3LYP/6-311+G**	0.817	0.775
PBE0/6-311+G**//B3LYP/6-311+G**	0.798	0.789

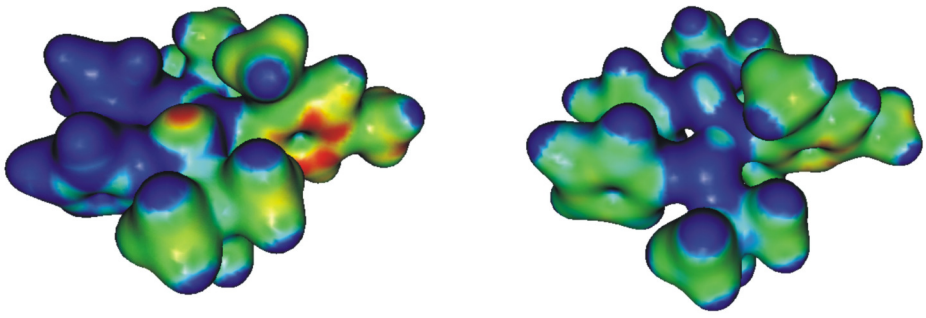


3^+ **$(FeCp(C_5H_4))_2PPh^+$**

Figure S16. Spin density maps of **3^+** and **$(FeCp(C_5H_4))_2PPh^+$** (B3LYP/6-311+G**). The spin density was drawn at the isovalue of 0.0004 e $bohr^{-3}$. While in case of **3^+** the spin density localised only at the ferrocene unit in case of **Fc_2PPh^+** the phosphorus atom has a small contribution to the spin density.

Table S4. The SCF energy differences between **3** and **3_{cis}** (ΔE(**3**-**3_{cis}**)) and between **3^+** and **3_{cis}^+** (ΔE(**3^+**-**3_{cis}^+**)) and the related inversion barriers (T_{invers}). Our attempts to localize the transition state of the inversion of the phosphorus in case of **3^+** at B3LYP/6-311+G** level of theory failed, due to convergence problems. On the other hand the results at B3LYP/6-31G* are similar to the results at B3LYP/6-311+G** level of theory.

level of theory	ΔE(**3**-**3_{cis}**)	TS_{invers}
B3LYP/6-311+G**	-2.8	5.0
B3LYP/6-31G*	-3.3	5.4
	ΔE(**3^+**-**3_{cis}^+**)	TS_{invers}
B3LYP/6-311+G**	-3.6	-
B3LYP/6-31G*	-5.1	5.7



3^+ 3_{cis}^+

Figure S17. The electrostatic potential map of $\mathbf{3}^+$ and $\mathbf{3}_{cis}^+$ (red <0.10, yellow 0.12, green 0.15, light blue 0.18, deep blue >0.20). While in case of $\mathbf{3}^+$ the positive charge is rather localized at the ferrocene unit, in case of $\mathbf{3}_{cis}^+$ the phosphorus atoms have partial positive charge

XYZ coordinates of the investigated systems

3

E(B3LYP/6-311+G**)= -3022.7937971

C	-4.221316	1.782669	-0.008593
C	-3.829580	1.452987	1.322259
C	-2.409992	1.362912	1.356659
C	-1.902938	1.625250	0.036187
C	-3.043670	1.895603	-0.797244
Fe	-3.129532	-0.004921	-0.001472
C	-3.037822	-1.904801	0.794877
C	-1.896657	-1.630295	-0.036592
C	-2.402344	-1.370193	-1.358040
C	-3.821638	-1.465765	-1.326155
C	-4.214474	-1.796643	0.004085
P	-0.185577	-1.555365	0.600006
C	0.588908	-3.234294	0.080173
C	-0.336853	-4.333728	0.637835
P	-0.190610	1.557215	-0.597849
C	0.577056	3.238140	-0.074312
C	1.961316	3.383167	-0.729776
B	0.730191	0.002254	0.000732
C	2.314742	0.004093	-0.000081
C	3.042270	-0.059780	-1.214003
C	4.438758	-0.066131	-1.192635
C	5.162883	0.009728	-0.002681
C	4.441266	0.086723	1.187175
C	3.043504	0.073093	1.211146
C	2.356768	-0.083273	-2.564251
C	2.361448	0.101199	2.563030
C	6.672387	-0.018060	-0.005269
C	1.971648	-3.373887	0.739993
C	0.712603	-3.404607	-1.442368
C	0.695768	3.407263	1.448766
C	-0.350755	4.335102	-0.633495

H	-1.812317	1.089451	2.212767
H	-4.496223	1.273977	2.153053
H	-5.235481	1.900875	-0.360345
H	-3.002053	2.107361	-1.855290
H	-2.997303	-2.115987	1.853079
H	-5.228818	-1.918567	0.354037
H	-4.487496	-1.289538	-2.158166
H	-1.804137	-1.094605	-2.213088
H	4.975270	-0.122361	-2.136314
H	4.979255	0.154184	2.129104
H	2.966832	0.647155	3.291395
H	1.374065	0.562659	2.524429
H	2.216749	-0.912314	2.950737
H	2.970193	-0.608097	-3.301253
H	1.378656	-0.564556	-2.528680
H	2.190439	0.931959	-2.938179
H	7.080432	0.423717	0.906779
H	7.046876	-1.045902	-0.068346
H	7.080561	0.528885	-0.859198
H	1.062518	4.415251	1.680372
H	-0.270139	3.287715	1.945111
H	1.398392	2.693851	1.880777
H	2.364596	4.376004	-0.499547
H	2.671664	2.640749	-0.365736
H	1.898699	3.294562	-1.817706
H	0.082349	5.317947	-0.415581
H	-0.464904	4.251902	-1.717811
H	-1.344719	4.301684	-0.182329
H	1.083340	-4.411609	-1.671946
H	-0.252288	-3.288858	-1.941622
H	1.414124	-2.689321	-1.873133
H	0.100044	-5.315378	0.422119
H	-0.454335	-4.249822	1.721745
H	-1.329632	-4.303964	0.183834
H	2.378830	-4.365824	0.512706
H	2.680487	-2.629644	0.376792
H	1.905429	-3.283429	1.827550

E(B3LYP/6-31G*)= -3022.375237

C	-3.816419	-1.419429	-1.335481
C	-4.217034	-1.761159	-0.008757
C	-3.042496	-1.885677	0.785458
C	-1.893915	-1.611461	-0.038732
C	-2.394661	-1.335034	-1.360670
Fe	-3.121179	-0.004526	-0.001689
C	-3.047300	1.877138	-0.788347
C	-1.899509	1.606701	0.038211
C	-2.402127	1.328298	1.359020
C	-3.824120	1.407751	1.330796
C	-4.223095	1.748352	0.003299
P	-0.189133	1.557234	-0.602797
C	0.564623	3.237497	-0.055869
C	0.660727	3.392296	1.471083
P	-0.184966	-1.555578	0.605461
C	0.575716	-3.234061	0.062817
C	1.965607	-3.390472	0.706183

B	0.736464	0.001911	0.000883
C	2.321478	0.003236	-0.000379
C	3.052657	0.042804	1.214323
C	4.452023	0.058647	1.189815
C	5.174630	0.009049	-0.003307
C	4.449306	-0.038495	-1.196159
C	3.050918	-0.030817	-1.217614
C	2.370164	0.036879	2.567963
C	2.364774	-0.020065	-2.569454
C	6.685149	-0.016861	-0.005937
C	-0.361124	4.335532	-0.619246
C	1.959051	3.396584	-0.688622
C	0.683688	-3.387567	-1.463448
C	-0.351736	-4.334476	0.618549
H	-1.797423	1.054908	2.213561
H	-4.487761	1.220286	2.165481
H	-5.241260	1.868786	-0.344156
H	-3.010995	2.104859	-1.845942
H	-3.007650	-2.112964	1.843195
H	-5.235509	-1.884967	0.336594
H	-4.478949	-1.234442	-2.171596
H	-1.789058	-1.059668	-2.213935
H	4.987069	-0.072088	-2.142662
H	4.991655	0.103504	2.134643
H	3.012901	0.491949	3.329655
H	1.417540	0.574439	2.562439
H	2.145973	-0.985365	2.896688
H	3.010186	-0.461838	-3.336637
H	1.418067	-0.568109	-2.565869
H	2.128229	1.002318	-2.888744
H	7.094730	0.414411	0.913695
H	7.067358	-1.043915	-0.082363
H	7.095521	0.542577	-0.854154
H	1.014892	4.402657	1.721970
H	-0.312611	3.254952	1.953525
H	1.366555	2.678668	1.904910
H	2.353478	4.392909	-0.446817
H	2.669923	2.655639	-0.315437
H	1.916601	3.313110	-1.780568
H	0.061073	5.321662	-0.383239
H	-0.456861	4.264008	-1.708679
H	-1.364957	4.290380	-0.185196
H	1.041927	-4.396952	-1.712540
H	-0.286332	-3.252048	-1.953112
H	1.391199	-2.671997	-1.891264
H	0.074763	-5.319495	0.385660
H	-0.456276	-4.263528	1.707223
H	-1.352200	-4.291641	0.176615
H	2.364605	-4.385408	0.466154
H	2.677317	-2.647029	0.339605
H	1.914237	-3.308422	1.797849

E(ωB97X-D/ 6-311+G**)= -3022.4434909

C	3.246624	0.030157	-1.001160
C	2.204645	0.004532	-0.053858
C	2.524918	-0.026639	1.310509

C	3.861630	-0.031833	1.710993
C	4.896883	-0.005266	0.787640
C	4.566013	0.027085	-0.567677
B	0.682321	0.007908	-0.449711
P	-0.208986	1.606414	-0.976973
C	0.620602	3.192723	-0.369412
C	1.912093	3.375142	-1.179482
C	1.447131	-0.038108	2.371900
C	6.338842	-0.030182	1.222372
C	2.940260	0.039923	-2.477463
C	-1.850374	1.622357	-0.190433
C	-3.086971	1.704953	-0.903511
C	-4.151863	1.690397	0.034266
C	-3.588597	1.618481	1.338920
C	-2.175561	1.572280	1.204773
Fe	-3.000371	-0.002438	0.228352
C	-3.653471	-1.672328	1.215800
C	-2.235897	-1.645771	1.132495
C	-1.862765	-1.620721	-0.251128
C	-3.075576	-1.636774	-1.008797
C	-4.172651	-1.658010	-0.108743
P	-0.194026	-1.592241	-0.978908
C	0.624566	-3.182224	-0.368049
C	-0.318042	-4.327540	-0.767658
C	0.898037	-3.253203	1.136226
C	1.951039	-3.336484	-1.125690
C	0.958225	3.232875	1.122555
C	-0.347830	4.337028	-0.703799
H	-3.130801	-1.599446	-2.086730
H	-5.217814	-1.639564	-0.379168
H	-4.234938	-1.667670	2.125853
H	-1.555634	-1.607618	1.969319
H	-3.179398	1.735627	-1.979066
H	-5.205859	1.707680	-0.199717
H	-4.139467	1.567428	2.266394
H	-1.464881	1.473406	2.011283
H	1.329470	-4.231492	1.380578
H	1.613821	-2.491273	1.444630
H	-0.016457	-3.144599	1.722238
H	2.396367	-4.308017	-0.883659
H	1.800170	-3.295939	-2.208137
H	2.669233	-2.563367	-0.843807
H	0.149503	-5.286631	-0.518711
H	-1.272400	-4.268945	-0.237746
H	-0.523957	-4.320002	-1.841972
H	1.376050	4.214831	1.375783
H	0.073410	3.083121	1.744641
H	1.706471	2.481178	1.375130
H	2.359325	4.345696	-0.936616
H	2.648871	2.604059	-0.943559
H	1.717152	3.353943	-2.255397
H	0.124305	5.295205	-0.460022
H	-0.603801	4.347251	-1.767377
H	-1.276058	4.261894	-0.131363
H	4.092564	-0.056545	2.773317
H	5.363315	0.049319	-1.306227

H	6.924993	0.722526	0.688547
H	6.791728	-1.004880	1.015761
H	6.435921	0.161302	2.293070
H	2.500682	-0.911877	-2.790938
H	2.217957	0.820011	-2.732324
H	3.844331	0.205267	-3.066735
H	1.414774	0.913930	2.909602
H	0.454585	-0.206535	1.944258
H	1.628244	-0.825140	3.108947

3_{cis} (not observed (*cis* type) isomer of **3**)
E(B3LYP/6-311+G**)= -3022.7893742

C	1.897946	1.635427	-0.191997
C	3.021892	1.688534	-1.085480
C	4.217780	1.709688	-0.316176
C	3.854207	1.685981	1.062788
C	2.432750	1.638256	1.144057
Fe	3.103563	-0.000489	0.110691
C	3.022414	-1.692064	-1.081723
C	1.896948	-1.635911	-0.190328
C	2.429384	-1.636267	1.146648
C	3.850925	-1.685473	1.068033
C	4.216921	-1.712648	-0.310243
P	0.157823	-1.614445	-0.757946
C	-0.592238	-3.252643	-0.106931
C	-1.983973	-3.431708	-0.741221
P	0.157962	1.614462	-0.756802
C	-0.590844	3.253168	-0.105986
C	0.331214	4.378264	-0.618668
B	-0.737710	0.000115	-0.268379
C	-2.307954	0.000273	-0.059603
C	-3.217012	0.000199	-1.151638
C	-4.589039	0.000176	-0.909404
C	-5.119125	0.000182	0.385814
C	-4.222934	0.000170	1.448362
C	-2.836236	0.000255	1.246942
C	-2.732745	0.000167	-2.584935
C	-1.948698	0.000397	2.475653
C	-6.612193	0.000898	0.608755
C	-0.704310	3.351392	1.423452
C	-1.983516	3.432075	-0.738251
C	-0.708016	-3.349739	1.422387
C	0.330315	-4.378304	-0.617431
H	2.953537	1.682228	-2.163038
H	5.224743	1.717713	-0.706078
H	4.537793	1.675816	1.898968
H	1.855586	1.580096	2.053570
H	2.955969	-1.688027	-2.159412
H	5.224574	-1.722469	-0.698327
H	4.533046	-1.674041	1.905395
H	1.850586	-1.575627	2.054956
H	-1.099427	4.337400	1.698682
H	-1.383184	2.599891	1.825720
H	0.266287	3.241908	1.910664
H	-2.380911	4.414188	-0.457421
H	-1.935954	3.391539	-1.829610

H	-2.691090	2.675796	-0.397067
H	-0.094295	5.348463	-0.338024
H	1.333398	4.315948	-0.188899
H	0.425819	4.354626	-1.707549
H	-1.103153	-4.335697	1.697785
H	0.261793	-3.239498	1.911010
H	-1.387834	-2.598209	1.822993
H	-2.382274	-4.413309	-0.459877
H	-2.691796	-2.674731	-0.402100
H	-1.934582	-3.392488	-1.832552
H	-0.096073	-5.348220	-0.337132
H	0.426921	-4.355225	-1.706154
H	1.331741	-4.316168	-0.185881
H	-4.604197	0.000008	2.466499
H	-5.269187	0.000052	-1.757048
H	-7.079387	0.885340	0.163928
H	-7.082079	-0.876031	0.152100
H	-6.855570	-0.005763	1.673348
H	-2.115849	0.876375	-2.801537
H	-2.114682	-0.875313	-2.801120
H	-3.576077	-0.000550	-3.278506
H	-2.141384	-0.877195	3.100519
H	-0.887184	-0.000830	2.220046
H	-2.139623	0.879428	3.099048

E(B3LYP/6-31G*)= -3022.370011

C	3.804374	-1.655985	1.133350
C	4.219676	-1.673434	-0.232713
C	3.051405	-1.658984	-1.046417
C	1.892856	-1.617459	-0.195259
C	2.379094	-1.619156	1.160930
Fe	3.081774	0.000503	0.155654
C	2.374142	1.615704	1.164669
C	1.891587	1.618010	-0.192822
C	3.052380	1.664007	-1.040696
C	4.218429	1.677244	-0.223732
C	3.799434	1.654454	1.141142
P	0.173580	1.609514	-0.823090
C	-0.594727	3.251001	-0.200752
C	-0.836152	3.324033	1.315487
P	0.173501	-1.609261	-0.821610
C	-0.593808	-3.251170	-0.199523
C	-0.834363	-3.324814	1.316837
B	-0.730078	0.000143	-0.312902
C	-2.290754	0.000023	-0.046563
C	-2.768033	-0.001081	1.283122
C	-4.147500	-0.002731	1.537798
C	-5.086199	-0.002501	0.509744
C	-4.607464	-0.002007	-0.807413
C	-3.243651	-0.000439	-1.103149
C	-1.831732	-0.001361	2.477979
C	-2.809539	-0.000178	-2.554154
C	-6.570121	0.002950	0.793394
C	-1.929427	3.455899	-0.944262
C	0.379029	4.373076	-0.616241
C	0.380065	-4.372769	-0.616032

C	-1.928920	-3.456236	-0.942287
H	3.027112	1.666379	-2.122711
H	5.242441	1.688637	-0.574528
H	4.450160	1.647189	2.006491
H	1.757862	1.567486	2.052106
H	3.023127	-1.657740	-2.128358
H	5.242733	-1.682230	-0.586346
H	4.457438	-1.650880	1.996947
H	1.765303	-1.574828	2.050294
H	-1.220402	4.319320	1.582010
H	-1.575808	2.587551	1.638162
H	0.086761	3.167642	1.882573
H	-2.355131	4.429461	-0.665360
H	-1.787464	3.451984	-2.030732
H	-2.663980	2.686866	-0.690048
H	-0.062951	5.347113	-0.366477
H	1.338611	4.297788	-0.095080
H	0.575254	4.360040	-1.694272
H	-1.218056	-4.320354	1.583199
H	0.088764	-3.168207	1.883506
H	-1.574160	-2.588763	1.640148
H	-2.354033	-4.430081	-0.663489
H	-2.663634	-2.687621	-0.687310
H	-1.787665	-3.451801	-2.028842
H	-0.061486	-5.347022	-0.366368
H	0.575610	-4.359256	-1.694177
H	1.339943	-4.297391	-0.095436
H	-4.490273	-0.004718	2.571898
H	-5.321651	-0.003615	-1.629476
H	-7.043560	0.925787	0.434054
H	-7.077451	-0.831482	0.293398
H	-6.772050	-0.077386	1.866364
H	-2.203047	0.880052	-2.796097
H	-2.194867	-0.875155	-2.794312
H	-3.677353	-0.004759	-3.221517
H	-1.997030	-0.880207	3.113150
H	-0.778570	-0.004204	2.179606
H	-1.992920	0.880236	3.110414

E(ωB97X-D/ 6-311+G**)= -3022.4398367

C	3.246624	0.030157	-1.001160
C	2.204645	0.004532	-0.053858
C	2.524918	-0.026639	1.310509
C	3.861630	-0.031833	1.710993
C	4.896883	-0.005266	0.787640
C	4.566013	0.027085	-0.567677
B	0.682321	0.007908	-0.449711
P	-0.208986	1.606414	-0.976973
C	0.620602	3.192723	-0.369412
C	1.912093	3.375142	-1.179482
C	1.447131	-0.038108	2.371900
C	6.338842	-0.030182	1.222372
C	2.940260	0.039923	-2.477463
C	-1.850374	1.622357	-0.190433
C	-3.086971	1.704953	-0.903511
C	-4.151863	1.690397	0.034266

C	-3.588597	1.618481	1.338920
C	-2.175561	1.572280	1.204773
Fe	-3.000371	-0.002438	0.228352
C	-3.653471	-1.672328	1.215800
C	-2.235897	-1.645771	1.132495
C	-1.862765	-1.620721	-0.251128
C	-3.075576	-1.636774	-1.008797
C	-4.172651	-1.658010	-0.108743
P	-0.194026	-1.592241	-0.978908
C	0.624566	-3.182224	-0.368049
C	-0.318042	-4.327540	-0.767658
C	0.898037	-3.253203	1.136226
C	1.951039	-3.336484	-1.125690
C	0.958225	3.232875	1.122555
C	-0.347830	4.337028	-0.703799
H	-3.130801	-1.599446	-2.086730
H	-5.217814	-1.639564	-0.379168
H	-4.234938	-1.667670	2.125853
H	-1.555634	-1.607618	1.969319
H	-3.179398	1.735627	-1.979066
H	-5.205859	1.707680	-0.199717
H	-4.139467	1.567428	2.266394
H	-1.464881	1.473406	2.011283
H	1.329470	-4.231492	1.380578
H	1.613821	-2.491273	1.444630
H	-0.016457	-3.144599	1.722238
H	2.396367	-4.308017	-0.883659
H	1.800170	-3.295939	-2.208137
H	2.669233	-2.563367	-0.843807
H	0.149503	-5.286631	-0.518711
H	-1.272400	-4.268945	-0.237746
H	-0.523957	-4.320002	-1.841972
H	1.376050	4.214831	1.375783
H	0.073410	3.083121	1.744641
H	1.706471	2.481178	1.375130
H	2.359325	4.345696	-0.936616
H	2.648871	2.604059	-0.943559
H	1.717152	3.353943	-2.255397
H	0.124305	5.295205	-0.460022
H	-0.603801	4.347251	-1.767377
H	-1.276058	4.261894	-0.131363
H	4.092564	-0.056545	2.773317
H	5.363315	0.049319	-1.306227
H	6.924993	0.722526	0.688547
H	6.791728	-1.004880	1.015761
H	6.435921	0.161302	2.293070
H	2.500682	-0.911877	-2.790938
H	2.217957	0.820011	-2.732324
H	3.844331	0.205267	-3.066735
H	1.414774	0.913930	2.909602
H	0.454585	-0.206535	1.944258
H	1.628244	-0.825140	3.108947

$TS_{3invers}$

E(B3LYP/6-311+G**)= -3022.785751

C	-2.975559	0.055305	1.204520

C	-2.348319	0.029343	-0.059759
C	-3.170617	0.029398	-1.216091
C	-4.558650	0.038131	-1.083319
C	-5.185485	0.036197	0.166189
C	-4.373068	0.047904	1.296004
B	-0.768603	-0.011354	-0.176549
P	0.134598	-1.630289	-0.770051
C	-0.657390	-3.219954	-0.027183
C	-2.031432	-3.421892	-0.693061
C	-2.576458	0.031930	-2.607305
C	-6.690749	0.005059	0.277973
C	-2.185367	0.143386	2.493779
C	1.836149	-1.660967	-0.073638
C	2.306403	-1.488409	1.274822
C	3.724212	-1.625105	1.283847
C	4.151367	-1.884900	-0.051856
C	2.996551	-1.913963	-0.881415
Fe	3.131427	-0.066236	0.044005
C	4.196226	1.674706	0.487595
C	2.851071	1.761883	0.940925
C	1.977645	1.601899	-0.192335
C	2.819427	1.428681	-1.346813
C	4.176006	1.465046	-0.922885
P	0.171692	1.553499	-0.154590
C	-0.489477	3.323139	0.032664
C	-0.161745	3.864960	1.437823
C	-2.008988	3.353618	-0.192818
C	0.200296	4.203895	-1.027982
C	-0.819777	-3.220975	1.499828
C	0.261607	-4.387218	-0.439910
H	2.530502	1.886053	1.964016
H	1.690248	-1.251921	2.128468
H	4.366882	-1.520035	2.145699
H	5.173252	-2.010197	-0.377995
H	2.981407	-2.064869	-1.950532
H	5.078855	1.727773	1.107565
H	5.040921	1.331730	-1.555552
H	2.466843	1.261971	-2.353302
H	-5.170505	0.043983	-1.981448
H	-4.833561	0.057699	2.280494
H	-2.686849	-0.400371	3.299009
H	-1.173656	-0.249266	2.390646
H	-2.088828	1.185674	2.819600
H	-2.037982	-0.896173	-2.817010
H	-3.356639	0.147862	-3.362729
H	-1.853665	0.843208	-2.733151
H	-7.156934	0.711464	-0.414811
H	-7.083485	-0.989279	0.038740
H	-7.020503	0.255381	1.288741
H	-1.226503	-4.186455	1.826998
H	0.135881	-3.081030	2.009527
H	-1.510390	-2.445117	1.830742
H	-2.454466	-4.378903	-0.365672
H	-2.739046	-2.636340	-0.425146
H	-1.946360	-3.451295	-1.782867
H	-0.195741	-5.334564	-0.131608

H	0.405475	-4.420891	-1.523509
H	1.244722	-4.322317	0.031463
H	-0.140052	5.239581	-0.914186
H	1.287334	4.196108	-0.921523
H	-0.046008	3.875038	-2.040404
H	-0.526799	4.895086	1.528711
H	-0.637837	3.267018	2.217971
H	0.914442	3.879277	1.624671
H	-2.351700	4.391596	-0.115741
H	-2.280494	2.982268	-1.182544
H	-2.550476	2.764434	0.547304

E(B3LYP/6-31G*)= -3022.366586

C	4.175928	1.365621	-0.975783
C	4.205832	1.648998	0.423150
C	2.862417	1.780490	0.876562
C	1.979460	1.578012	-0.245210
C	2.815416	1.331688	-1.392247
Fe	3.116915	-0.068395	0.067422
C	3.021317	-1.936847	-0.766863
C	1.825106	-1.641628	-0.024982
C	2.238639	-1.397078	1.332733
C	3.656093	-1.528684	1.410697
C	4.140708	-1.861201	0.109549
P	0.153447	-1.629768	-0.789690
C	-0.652777	-3.226534	-0.077391
C	0.303705	-4.385492	-0.425648
P	0.172084	1.552446	-0.215553
C	-0.476531	3.324194	-0.007588
C	0.190239	4.197334	-1.090672
B	-0.768916	-0.017496	-0.195108
C	-2.345994	0.025852	-0.054653
C	-2.950331	0.087502	1.224408
C	-4.346279	0.085966	1.342339
C	-5.182104	0.044241	0.225995
C	-4.579274	0.014561	-1.035630
C	-3.190869	0.001357	-1.195107
C	-2.126560	0.212806	2.490539
C	-2.620722	-0.020138	-2.597843
C	-6.685623	0.012871	0.370967
C	-1.984708	-3.453014	-0.819100
C	-0.901693	-3.214174	1.438251
C	-0.111268	3.872919	1.386160
C	-2.002775	3.359166	-0.194941
H	2.548222	1.965313	1.895121
H	1.584531	-1.118969	2.148370
H	4.262000	-1.379231	2.295597
H	5.177340	-2.009048	-0.165256
H	3.052641	-2.152547	-1.827079
H	5.093891	1.727137	1.037256
H	5.038279	1.191489	-1.606567
H	2.454894	1.123786	-2.390963
H	-5.209408	0.001021	-1.923595
H	-4.789425	0.125147	2.336260
H	-2.706059	-0.093459	3.368268
H	-1.214617	-0.390489	2.458348

H	-1.807729	1.250756	2.655363
H	-2.067438	-0.944495	-2.798876
H	-3.416652	0.064039	-3.345007
H	-1.914353	0.803214	-2.757861
H	-7.002917	0.400650	1.344786
H	-7.176846	0.608412	-0.407019
H	-7.073709	-1.011136	0.284939
H	-1.295415	-4.189151	1.760890
H	0.020819	-3.032248	1.999670
H	-1.637862	-2.455357	1.715618
H	-2.421403	-4.410320	-0.502468
H	-2.714715	-2.667934	-0.604294
H	-1.835731	-3.497684	-1.904098
H	-0.159822	-5.339049	-0.137828
H	0.514895	-4.426903	-1.500477
H	1.257654	-4.304624	0.105109
H	-0.134837	5.239717	-0.969927
H	1.282428	4.177162	-1.016634
H	-0.089584	3.868125	-2.096792
H	-0.471900	4.906583	1.482902
H	-0.568730	3.280254	2.185076
H	0.971936	3.885714	1.544962
H	-2.340358	4.401911	-0.125969
H	-2.303180	2.971517	-1.173000
H	-2.529143	2.783521	0.570234

E(ωB97X-D/6-311+G**)= -3022.4341177

C	4.146125	1.369366	-0.988684
C	4.177141	1.669198	0.402372
C	2.839778	1.810574	0.853174
C	1.964750	1.595849	-0.262179
C	2.790567	1.334689	-1.403326
Fe	3.090923	-0.051408	0.072258
C	3.029530	-1.932529	-0.729770
C	1.817024	-1.633786	-0.032599
C	2.178482	-1.364886	1.326932
C	3.587495	-1.485486	1.453066
C	4.115133	-1.835036	0.178202
P	0.177094	-1.629176	-0.837803
C	-0.645637	-3.167370	-0.092188
C	0.293036	-4.345474	-0.392321
P	0.171733	1.525068	-0.195333
C	-0.522542	3.251898	-0.015365
C	0.116533	4.130886	-1.101123
B	-0.737023	-0.035496	-0.242280
C	-2.306376	-0.000981	-0.070227
C	-2.875541	0.059894	1.210727
C	-4.263578	0.068298	1.355989
C	-5.112764	0.041064	0.258530
C	-4.537835	0.006021	-1.011032
C	-3.160725	-0.019909	-1.191380
C	-2.024464	0.185566	2.452320
C	-2.597312	-0.059592	-2.589297
C	-6.609901	0.048419	0.422552
C	-1.975753	-3.391976	-0.824959
C	-0.902215	-3.099529	1.414697

C	-0.174517	3.820018	1.367711
C	-2.043258	3.232202	-0.201862
H	2.523542	1.995527	1.868867
H	1.495371	-1.060585	2.105978
H	4.161778	-1.305365	2.349944
H	5.159682	-1.970948	-0.059463
H	3.095526	-2.153058	-1.785088
H	5.063636	1.741791	1.014554
H	5.005207	1.173227	-1.612763
H	2.424940	1.102726	-2.392471
H	-5.185347	-0.003820	-1.884403
H	-4.688818	0.107398	2.355728
H	-2.526338	-0.251176	3.319210
H	-1.050848	-0.293163	2.339277
H	-1.833006	1.241088	2.675287
H	-2.087962	-1.008063	-2.782313
H	-3.385295	0.060687	-3.335485
H	-1.854295	0.729829	-2.738435
H	-7.062861	0.870441	-0.138955
H	-7.050061	-0.882300	0.052345
H	-6.893279	0.159222	1.471324
H	-1.298128	-4.060410	1.765959
H	0.015886	-2.898930	1.972010
H	-1.639820	-2.333497	1.656191
H	-2.422772	-4.333304	-0.485029
H	-2.692106	-2.592834	-0.622928
H	-1.828036	-3.462394	-1.906632
H	-0.180650	-5.279575	-0.069873
H	0.505378	-4.426498	-1.462595
H	1.244533	-4.249895	0.137322
H	-0.247821	5.158899	-0.995506
H	1.206311	4.149612	-1.015493
H	-0.142587	3.775907	-2.101804
H	-0.582620	4.832921	1.463094
H	-0.596172	3.206669	2.167488
H	0.906872	3.883245	1.514106
H	-2.413102	4.262591	-0.161953
H	-2.328160	2.804636	-1.165637
H	-2.548918	2.660793	0.578123

A

E(B3LYP/6-311+G**)= -710.6118452

B	0.000000	0.000000	0.000000
P	0.000000	0.000000	1.891719
P	1.552468	0.000000	-1.080762
H	-1.019943	0.306988	-0.532593
H	2.331489	-1.043693	-0.522789
H	1.071675	-0.689011	-2.220298
H	-1.209909	-0.689281	2.147990
H	0.903029	-1.043663	2.212143

B

E(B3LYP/6-311+G**)= -1984.1286658

C	-0.742259	2.894849	1.555535
C	-0.474515	2.933393	0.178776
C	0.100447	4.092608	-0.357067

C	0.413037	5.178464	0.460546
C	0.141940	5.126402	1.825243
C	-0.440728	3.982728	2.371071
P	-0.852661	1.535115	-0.961166
C	-2.660567	1.225126	-0.868502
C	-3.542971	2.035081	-0.140471
C	-4.920413	1.828063	-0.210867
C	-5.442718	0.813514	-1.008674
C	-4.574441	0.011920	-1.749585
C	-3.201136	0.222426	-1.690230
B	0.308986	0.084059	-0.551530
C	1.829950	0.487180	-0.417114
C	2.614696	0.847623	-1.536584
C	3.956336	1.201286	-1.357323
C	4.557602	1.218493	-0.100686
C	3.778062	0.850557	0.996714
C	2.440819	0.479885	0.859959
C	2.057235	0.852046	-2.945650
C	6.011810	1.586671	0.070269
C	1.665592	0.074801	2.092606
P	-0.166762	-1.740076	-0.873937
C	1.186307	-2.820937	-0.232949
C	2.404715	-2.845820	-0.928308
C	3.444805	-3.672195	-0.512621
C	3.280770	-4.508355	0.591164
C	2.067985	-4.506839	1.276491
C	1.029223	-3.669361	0.871168
C	-1.647905	-2.223796	0.111729
C	-2.435144	-3.281945	-0.365183
C	-3.553402	-3.715684	0.343289
C	-3.911525	-3.088176	1.535292
C	-3.142439	-2.030400	2.016633
C	-2.017013	-1.605160	1.313373
H	4.224558	0.843519	1.987428
H	4.546881	1.468525	-2.229411
H	1.437412	1.733364	-3.132103
H	2.867033	0.852205	-3.678824
H	1.426362	-0.019125	-3.141053
H	1.201953	-0.907652	1.965404
H	2.319950	0.020370	2.965213
H	0.872963	0.793405	2.319715
H	6.399657	2.098766	-0.813208
H	6.157576	2.242690	0.932997
H	6.628045	0.695583	0.233248
H	-2.169055	-3.766894	-1.298272
H	-4.148099	-4.537708	-0.039723
H	-4.785698	-3.419902	2.084348
H	-3.416762	-1.536508	2.942344
H	-1.421914	-0.787621	1.700976
H	2.543619	-2.216471	-1.799501
H	4.381418	-3.669199	-1.059340
H	4.087949	-5.158744	0.909016
H	1.926336	-5.156338	2.133685
H	0.094214	-3.680700	1.417999
H	-3.162207	2.837932	0.477594
H	-5.584716	2.466636	0.361515

H	-6.513727	0.653600	-1.060553
H	-4.967266	-0.775210	-2.383616
H	-2.545300	-0.394719	-2.294273
H	0.306275	4.143790	-1.419889
H	0.864194	6.064596	0.028217
H	0.381261	5.971251	2.461366
H	-0.655079	3.935286	3.433217
H	-1.196345	2.012708	1.991422

C

E(B3LYP/6-311+G**)=-1452.945595

C	-4.040877	-0.619188	-0.04791
C	-3.471693	-0.193897	-1.25008
C	-2.102996	0.043280	-1.38016
C	-1.238332	-0.154351	-0.27137
C	-1.807582	-0.607246	0.94093
C	-3.187128	-0.823154	1.03254
C	-1.570421	0.484830	-2.72483
B	0.301963	0.131330	-0.42023
P	1.651040	-1.051356	-0.60807
C	1.819168	-2.724380	0.24227
C	2.371638	-3.746776	-0.76976
C	-0.978462	-0.893589	2.17714
C	-5.530356	-0.829462	0.08245
P	1.170165	1.848951	-0.77867
C	0.673074	3.089481	0.59673
C	1.631258	4.291254	0.47964
C	2.919944	1.322710	-0.29224
C	3.411536	-0.967789	-1.16514
C	2.096358	-2.521908	1.74434
C	0.423938	-3.163674	0.71914
C	-0.759976	3.552453	0.27433
C	0.721704	2.529001	2.02468
H	3.673562	-0.927727	-2.22615
H	3.642483	2.038988	-0.69098
H	-3.600281	-1.165053	1.97851
H	-4.112933	-0.042791	-2.11399
H	-0.797231	-0.197346	-3.09162
H	-2.371080	0.520807	-3.46671
H	-1.109529	1.474767	-2.67365
H	-1.389461	-0.380499	3.05214
H	-0.983544	-1.965001	2.40747
H	0.060882	-0.588662	2.06126
H	-6.005486	-0.927642	-0.89623
H	-5.758221	-1.728847	0.66120
H	-6.003948	0.015238	0.59491
H	2.232864	-3.496395	2.22824
H	3.004654	-1.937849	1.91467
H	1.267385	-2.010181	2.23713
H	2.478952	-4.722386	-0.28209
H	1.701113	-3.866049	-1.62404
H	3.356157	-3.457360	-1.14657
H	0.506920	-4.126260	1.236058
H	-0.015610	-2.446952	1.41555
H	-0.265911	-3.286407	-0.11840
H	-1.081749	4.303525	1.00551

H	-0.817308	4.005662	-0.71911
H	-1.470822	2.723351	0.31248
H	0.507359	3.327497	2.74598
H	-0.021253	1.744172	2.16983
H	1.703259	2.120496	2.27953
H	1.322365	5.081862	1.17367
H	2.660731	4.019623	0.73021
H	1.627470	4.709495	-0.53071
H	4.248487	-1.426321	-0.63247
H	3.013281	1.316330	0.79739
H	3.575749	-0.040188	-1.71151
H	3.108030	0.311944	-0.651272

D

E(B3LYP/6-311+G**)= -1451.736386

C	2.027351	0.117358	1.207298
C	3.423486	0.110935	1.183077
C	4.145620	-0.035074	-0.001058
C	3.421549	-0.173685	-1.183330
C	2.024137	-0.154686	-1.207502
C	1.294038	-0.011184	-0.000760
C	5.654978	-0.015500	-0.001246
C	1.337768	-0.308251	-2.548812
B	-0.278604	0.001309	-0.000968
P	-1.372589	1.318587	-0.829901
C	-1.306867	3.039088	0.004910
C	-1.804850	3.010055	1.459112
C	1.342969	0.275444	2.549031
P	-1.396491	-1.295964	0.826568
C	-1.357106	-3.020162	-0.002003
C	-1.854502	-2.988274	-1.456388
C	-3.095938	-0.538033	0.520543
C	-3.084998	0.588118	-0.528548
C	0.152641	3.521340	-0.050146
C	-2.190221	3.994580	-0.820268
C	0.094658	-3.525048	0.054939
C	-2.255427	-3.959112	0.826104
H	-3.406678	0.198986	-1.497528
H	-3.814035	-1.319860	0.257531
H	3.961846	0.219947	2.120748
H	3.957780	-0.300317	-2.119767
H	0.823922	0.608402	-2.847373
H	2.063365	-0.559574	-3.325446
H	0.581424	-1.098217	-2.533865
H	2.072480	0.508920	3.327554
H	0.601606	1.079607	2.537818
H	0.811539	-0.632921	2.841949
H	6.035104	1.012134	0.016274
H	6.061031	-0.526360	0.875888
H	6.059935	-0.499343	-0.893121
H	-1.782010	4.022517	1.881367
H	-2.835428	2.652123	1.529716
H	-1.182771	2.370850	2.088509
H	-2.145123	5.003156	-0.392733
H	-1.855650	4.050971	-1.858907
H	-3.239304	3.685477	-0.819754

H	0.220893	4.532025	0.368347
H	0.820974	2.873678	0.520371
H	0.521809	3.560561	-1.078428
H	-1.849016	-4.002672	-1.874531
H	-2.878768	-2.612894	-1.528418
H	-1.221438	-2.362448	-2.088254
H	0.147179	-4.537311	-0.361939
H	0.773477	-2.888860	-0.516074
H	0.462486	-3.568602	1.083534
H	-2.224951	-4.969925	0.402573
H	-1.922637	-4.016489	1.865261
H	-3.299822	-3.634498	0.823400
H	-3.791383	1.381414	-0.268092
H	-3.414328	-0.143834	1.488514

D_{cis} (*cis* isomer of **D**)
E(B3LYP/6-311+G**)=-1451.737312

C	-2.113740	-0.257823	-1.345401
C	-1.267779	-0.165803	-0.206184
C	-1.866784	-0.194250	1.068644
C	-3.256579	-0.313361	1.195320
C	-4.090021	-0.404906	0.086468
C	-3.492023	-0.372018	-1.177541
B	0.287629	-0.024578	-0.399561
P	1.469504	-1.457686	-0.983919
C	1.693804	-2.744251	0.423627
C	0.331741	-3.419058	0.659926
C	-1.047581	-0.126062	2.339290
C	-5.587021	-0.537349	0.229470
C	-1.552319	-0.212726	-2.749550
P	1.276658	1.547119	-0.695074
C	0.916110	3.119031	0.313672
C	1.279636	2.977255	1.800337
C	2.983378	0.897953	-0.294899
C	3.081340	-0.464223	-1.010675
C	2.685208	-3.798779	-0.107719
C	2.238619	-2.159618	1.736794
C	1.756750	4.254705	-0.305086
C	-0.578803	3.446070	0.155788
H	3.315535	-0.300493	-2.065763
H	3.755313	1.579945	-0.662304
H	-3.691920	-0.332535	2.191159
H	-4.121179	-0.434697	-2.061470
H	-0.832101	-1.017606	-2.919452
H	-2.349822	-0.307317	-3.489419
H	-1.024938	0.726889	-2.940536
H	-1.007821	-1.100064	2.838978
H	-0.019251	0.182554	2.145892
H	-1.481744	0.581296	3.052148
H	-5.940467	-1.492323	-0.173047
H	-5.893139	-0.483455	1.276460
H	-6.110186	0.255215	-0.314613
H	2.374809	-2.961030	2.473986
H	3.211940	-1.683474	1.593998
H	1.560003	-1.423502	2.169263
H	2.826040	-4.585677	0.642822

H	2.317350	-4.264950	-1.024806
H	3.668568	-3.369499	-0.319547
H	0.444771	-4.231524	1.387252
H	-0.412618	-2.721720	1.046747
H	-0.063515	-3.850818	-0.263414
H	-0.801218	4.391256	0.664015
H	-0.853814	3.560943	-0.896179
H	-1.215280	2.670947	0.586269
H	1.110901	3.931992	2.313052
H	0.670425	2.222114	2.298091
H	2.332118	2.716572	1.939642
H	1.554736	5.193533	0.223504
H	2.829479	4.056675	-0.225411
H	1.517131	4.400659	-1.360971
H	3.896730	-1.066639	-0.601869
H	3.118981	0.789411	0.784537

E

E(B3LYP/6-311+G**)= -1491.0634276

C	1.931693	-0.404279	1.123181
C	1.176759	-0.215573	-0.055894
C	1.868147	-0.231996	-1.298194
C	3.248857	-0.419836	-1.328078
C	3.998869	-0.611104	-0.164468
C	3.316846	-0.599874	1.047092
B	-0.388561	0.016809	-0.043058
P	-1.162857	1.602621	0.591409
C	-0.287710	3.256512	0.204046
C	-1.037035	4.365134	0.971381
C	1.145944	-0.055606	-2.617551
C	5.492638	-0.819136	-0.231277
C	1.307021	-0.434561	2.503397
P	-1.590177	-1.321076	-0.680464
C	-1.438482	-2.989830	0.239938
C	-1.691609	-2.875015	1.752083
C	-3.319458	-0.706049	-0.323340
C	-3.511752	0.712091	-0.883990
C	-2.936512	1.817638	0.009849
C	-2.477240	-3.946316	-0.379221
C	-0.029705	-3.551839	-0.019644
C	1.156882	3.184891	0.728291
C	-0.280590	3.582439	-1.299027
H	-4.010372	-1.390895	-0.820927
H	-3.559913	-0.721726	0.744591
H	-3.062604	0.773148	-1.881104
H	-4.583087	0.905231	-1.013798
H	-3.000963	2.774108	-0.514187
H	-3.554820	1.915382	0.906894
H	-0.533415	5.324886	0.809167
H	-2.071059	4.479929	0.636398
H	-1.048820	4.168401	2.046520
H	1.645147	4.153986	0.572687
H	1.183038	2.966258	1.798888
H	1.745262	2.424797	0.213602
H	0.165849	4.571044	-1.463021
H	0.306181	2.854653	-1.861724

H	-1.288563	3.608358	-1.722272
H	3.755968	-0.414131	-2.289508
H	3.874210	-0.740121	1.969710
H	0.059574	-4.541136	0.444192
H	0.162500	-3.666237	-1.089889
H	0.751668	-2.912927	0.394300
H	-2.375520	-4.939829	0.072480
H	-3.502338	-3.611224	-0.201499
H	-2.334203	-4.050230	-1.457957
H	-1.619999	-3.865933	2.217971
H	-0.962359	-2.224234	2.236087
H	-2.689768	-2.486712	1.970884
H	0.291650	-0.041274	2.512013
H	1.277490	-1.458448	2.893446
H	1.898557	0.156134	3.209102
H	1.850119	0.205316	-3.411124
H	0.627271	-0.971557	-2.913528
H	0.383567	0.725623	-2.569676
H	5.926648	-0.909283	0.766844
H	5.741616	-1.729095	-0.787006
H	5.988422	0.014365	-0.738869

E_{cis} (*cis* isomer of E)
E(B3LYP/6-311+G**)= -1491.061832

C	-3.761652	-1.385138	0.168011
C	-3.207824	-1.171969	-1.098509
C	-1.906600	-0.703655	-1.272653
C	-1.096521	-0.429209	-0.138206
C	-1.648832	-0.647772	1.140395
C	-2.962724	-1.114861	1.273331
C	-1.399907	-0.478081	-2.680481
B	0.377391	0.118678	-0.295266
P	0.794382	1.935263	-0.593864
C	-0.409509	3.246152	0.091944
C	-1.769089	3.050565	-0.602003
C	-0.849154	-0.429289	2.407862
C	-5.177689	-1.886915	0.318423
P	1.841569	-0.984727	-0.849323
C	2.018658	-2.623248	0.129528
C	3.137660	-3.429107	-0.562775
C	3.395360	-0.006118	-0.442856
C	3.258352	1.073582	0.642218
C	2.462774	2.304505	0.198555
C	-0.591322	3.188285	1.617185
C	0.160284	4.623533	-0.305544
C	2.380504	-2.427844	1.610997
C	0.702531	-3.409391	0.004202
H	4.157996	-0.733663	-0.155314
H	3.750096	0.450056	-1.372800
H	2.797155	0.638393	1.533679
H	4.261056	1.410192	0.935171
H	2.294793	2.957505	1.059377
H	3.050253	2.879277	-0.523203
H	-0.536552	5.410441	0.004720
H	1.120156	4.829984	0.175396
H	0.299067	4.702463	-1.386983

H	-2.461976	3.834001	-0.273863
H	-1.674788	3.121946	-1.688721
H	-2.214045	2.084635	-0.358705
H	-1.208067	4.032509	1.949619
H	-1.092631	2.270792	1.924719
H	0.361365	3.254016	2.149872
H	-3.364596	-1.271942	2.271153
H	-3.811944	-1.374308	-1.979036
H	2.513072	-3.404707	2.092721
H	3.317078	-1.877527	1.734029
H	1.599310	-1.892996	2.152239
H	3.260485	-4.394422	-0.058017
H	2.898988	-3.622018	-1.611395
H	4.103935	-2.918368	-0.526137
H	0.826300	-4.399731	0.458051
H	-0.127137	-2.909586	0.504471
H	0.422812	-3.556408	-1.042455
H	-1.205934	0.582202	-2.869587
H	-0.459346	-1.003201	-2.862287
H	-2.131582	-0.820865	-3.415120
H	-1.436012	0.107798	3.158780
H	-0.559049	-1.385723	2.856309
H	0.064583	0.139823	2.227713
H	-5.897094	-1.181181	-0.109545
H	-5.317491	-2.842160	-0.197396
H	-5.438269	-2.032810	1.368927

3^+

E(B3LYP/6-311+G**)= -3022.5659208

C	-3.792497	-1.543754	-1.38008
C	-4.208108	-1.858208	-0.05701
C	-3.042144	-1.931783	0.75856
C	-1.886596	-1.647237	-0.05338
C	-2.379784	-1.418018	-1.38267
Fe	-3.155472	-0.003864	-0.00164
C	-2.386842	1.412630	1.38111
C	-1.891493	1.643399	0.05292
C	-3.046142	1.924463	-0.76150
C	-4.213649	1.847194	0.05153
C	-3.799889	1.533943	1.37548
P	-0.175925	1.564845	-0.62558
C	0.577774	3.253236	-0.09595
C	0.728111	3.407082	1.42421
P	-0.172591	-1.563358	0.62841
C	0.586669	-3.250450	0.10271
C	-0.355023	-4.345393	0.64081
B	0.731452	0.001519	0.00096
C	2.307683	0.002830	-0.00011
C	3.032982	0.079072	1.21345
C	4.429471	0.093490	1.18744
C	5.150742	0.009411	-0.00315
C	4.426615	-0.074492	-1.19350
C	3.031281	-0.068419	-1.21649
C	2.353021	0.113697	2.56662
C	2.347610	-0.099734	-2.56792
C	6.658673	-0.015761	-0.00618

C	-0.363902	4.346364	-0.63784
C	1.947710	3.388777	-0.78440
C	1.953705	-3.382481	0.79757
C	0.744332	-3.404556	-1.41665
H	-1.775447	-1.126543	-2.22909
H	-4.444098	-1.383823	-2.22751
H	-5.227541	-2.004939	0.26880
H	-3.016020	-2.149137	1.81629
H	-3.018390	2.142047	-1.81914
H	-5.232828	1.990910	-0.27641
H	-4.452804	1.371983	2.22152
H	-1.783439	1.123004	2.22884
H	4.968322	0.167018	2.12767
H	4.963847	-0.136750	-2.13565
H	2.940705	-0.666025	-3.28961
H	1.352100	-0.545463	-2.52822
H	2.225905	0.910425	-2.97205
H	2.938782	0.697576	3.28036
H	1.349868	0.541645	2.52559
H	2.250473	-0.894125	2.98195
H	7.065032	0.516838	-0.86905
H	7.067652	0.437958	0.89866
H	7.029950	-1.045013	-0.05476
H	1.132277	-4.404652	-1.64010
H	-0.209267	-3.306958	-1.94256
H	1.446927	-2.679914	-1.82785
H	2.367306	-4.370494	0.57120
H	2.667814	-2.634576	0.45349
H	1.862325	-3.303171	1.88359
H	0.092819	-5.324657	0.44492
H	-0.505077	-4.260277	1.72017
H	-1.332196	-4.333569	0.15136
H	1.113494	4.407715	1.64966
H	-0.227749	3.307911	1.94566
H	1.429815	2.683415	1.83858
H	0.080727	5.326524	-0.43911
H	-0.508540	4.261615	-1.71795
H	-1.343419	4.331998	-0.15314
H	2.357737	4.377716	-0.55566
H	2.662264	2.642653	-0.43738
H	1.861576	3.309882	-1.870881

E(B3LYP/6-31G*)=-3022.155269

C	3.031289	-0.068424	-1.216510
C	2.307694	0.002829	-0.000130
C	3.032994	0.079083	1.213443
C	4.429483	0.093511	1.187426
C	5.150753	0.009431	-0.003177
C	4.426626	-0.074484	-1.193522
B	0.731463	0.001507	0.000953
P	-0.172582	-1.563362	0.628421
C	0.586675	-3.250464	0.102751
C	0.744343	-3.404594	-1.416623
C	2.353034	0.113713	2.566613
C	6.658684	-0.015731	-0.006210
C	2.347616	-0.099753	-2.567938

C	-1.886584	-1.647247	-0.053386
C	-3.042138	-1.931781	0.758561
C	-4.208097	-1.858208	-0.057025
C	-3.792477	-1.543768	-1.380091
C	-2.379763	-1.418048	-1.382670
Fe	-3.155472	-0.003867	-0.001661
C	-3.799919	1.533950	1.375447
C	-2.386871	1.412646	1.381108
C	-1.891505	1.643397	0.052926
C	-3.046145	1.924433	-0.761528
C	-4.213663	1.847165	0.051491
P	-0.175929	1.564856	-0.625569
C	0.577752	3.253253	-0.095935
C	1.947695	3.388803	-0.784365
C	0.728071	3.407102	1.424235
C	-0.363926	4.346373	-0.637831
C	-0.355021	-4.345397	0.640862
C	1.953710	-3.382489	0.797613
H	-1.775409	-1.126589	-2.229087
H	-4.444078	-1.383836	-2.227526
H	-5.227531	-2.004924	0.268796
H	-3.016022	-2.149128	1.816289
H	-3.018388	2.142002	-1.819172
H	-5.232841	1.990873	-0.276463
H	-4.452847	1.372000	2.221475
H	-1.783511	1.123033	2.228875
H	4.968335	0.167047	2.127652
H	4.963860	-0.136747	-2.135672
H	2.940712	-0.666046	-3.289629
H	1.352108	-0.545487	-2.528229
H	2.225903	0.910402	-2.972078
H	2.938793	0.697599	3.280344
H	1.349879	0.541656	2.525580
H	2.250491	-0.894107	2.981941
H	7.065034	0.516866	-0.869089
H	7.067667	0.437996	0.898632
H	7.029968	-1.044980	-0.054791
H	1.132286	-4.404694	-1.640058
H	-0.209254	-3.307001	-1.942532
H	1.446941	-2.679960	-1.827830
H	2.367308	-4.370507	0.571262
H	2.667821	-2.634591	0.453520
H	1.862326	-3.303163	1.883630
H	0.092819	-5.324665	0.444987
H	-0.505078	-4.260264	1.720214
H	-1.332193	-4.333578	0.151409
H	1.113444	4.407739	1.649689
H	-0.227794	3.307924	1.945680
H	1.429777	2.683441	1.838622
H	0.080693	5.326536	-0.439102
H	-0.508552	4.261621	-1.717946
H	-1.343448	4.332001	-0.153143
H	2.357713	4.377745	-0.555622
H	2.662251	2.642685	-0.437342
H	1.861574	3.309905	-1.870844

3_{cis}^{+}

E(B3LYP/6-31G*)= -3022.147066

C	-3.151407	-0.181025	-1.262830
C	-2.368951	-0.067375	-0.078670
C	-3.030691	0.019601	1.170245
C	-4.430151	0.002793	1.216031
C	-5.206834	-0.103560	0.061730
C	-4.542039	-0.193495	-1.169361
B	-0.803699	-0.023256	-0.147052
P	0.147772	1.586444	-0.400550
C	-0.683064	3.276440	-0.137373
C	-0.979034	3.493895	1.359336
C	-2.277463	0.076919	2.483682
C	-6.714014	-0.128501	0.126556
C	-2.507719	-0.274131	-2.628568
C	1.809952	1.614404	0.297216
C	2.235871	1.060677	1.564441
C	3.647983	1.203776	1.656143
C	4.114464	1.830178	0.464854
C	2.994272	2.086742	-0.372453
Fe	3.088646	0.074977	0.011367
C	4.277989	-1.618472	-0.201603
C	3.017115	-1.937379	0.374774
C	1.983910	-1.526605	-0.544262
C	2.650443	-0.945588	-1.690623
C	4.051776	-1.011476	-1.469496
P	0.198282	-1.601897	-0.356834
C	-0.370924	-3.290013	0.290177
C	-1.869338	-3.463294	-0.026716
C	-0.136184	-3.392456	1.811810
C	0.440702	-4.370931	-0.453691
C	0.300168	4.353194	-0.640380
C	-1.979508	3.332794	-0.965657
H	3.025996	2.531972	-1.358218
H	5.146276	2.052265	0.226162
H	4.263756	0.871375	2.481763
H	1.586999	0.617840	2.308256
H	2.156406	-0.539624	-2.563296
H	4.814387	-0.641641	-2.142344
H	5.242411	-1.788811	0.258698
H	2.865840	-2.385451	1.347034
H	-4.924437	0.073787	2.182821
H	-5.128898	-0.271104	-2.082161
H	-3.264606	-0.325849	-3.416091
H	-1.866496	0.590574	-2.841161
H	-1.871574	-1.164021	-2.721864
H	-2.214815	-0.917086	2.946634
H	-1.253026	0.445414	2.367582
H	-2.785994	0.725843	3.204530
H	-7.153687	0.616253	-0.546837
H	-7.105327	-1.106777	-0.179555
H	-7.076831	0.073569	1.138400
H	-1.387954	4.503372	1.495372
H	-1.718577	2.781817	1.735038
H	-0.073365	3.419032	1.970297
H	-2.424980	4.328010	-0.848069

H	-1.786915	3.182000	-2.033267
H	-2.715686	2.596282	-0.636115
H	-0.173258	5.335435	-0.525684
H	1.231328	4.366958	-0.066214
H	0.542914	4.225278	-1.701029
H	-0.485332	-4.373481	2.157649
H	0.922633	-3.311849	2.076310
H	-0.689491	-2.626495	2.363105
H	0.110921	-5.354885	-0.099752
H	0.274863	-4.332455	-1.535244
H	1.515394	-4.293126	-0.266922
H	-2.173369	-4.466143	0.296420
H	-2.495743	-2.737422	0.495875
H	-2.070838	-3.384856	-1.099503

E(B3LYP/6-311+G**)= -3022.5602074

C	-4.112726	1.305466	-1.232483
C	-4.228381	1.728271	0.121788
C	-2.921868	1.903909	0.650500
C	-1.974405	1.582074	-0.386304
C	-2.734295	1.214274	-1.558049
Fe	-3.117469	-0.051100	0.019167
C	-2.991222	-2.010312	-0.634574
C	-1.857672	-1.641272	0.171843
C	-2.361101	-1.279046	1.475775
C	-3.774111	-1.426025	1.453826
C	-4.161079	-1.869821	0.157423
P	-0.148646	-1.584528	-0.392761
C	0.659305	-3.283998	-0.132628
C	2.008697	-3.330883	-0.868585
P	-0.180512	1.589851	-0.284244
C	0.469690	3.302327	0.195003
C	-0.348314	4.341546	-0.597550
B	0.807508	0.012906	-0.133546
C	2.373786	0.039501	-0.061185
C	3.161019	0.128603	-1.240973
C	4.548855	0.134516	-1.140904
C	5.205889	0.057123	0.093440
C	4.423890	-0.026626	1.242665
C	3.025846	-0.033271	1.189505
C	2.525510	0.205712	-2.609765
C	2.268722	-0.076631	2.499871
C	6.711438	0.074463	0.165289
C	0.849461	-3.534258	1.375833
C	-0.291771	-4.341677	-0.725550
C	1.956764	3.414209	-0.186482
C	0.293236	3.525424	1.710805
H	-2.956473	-2.308250	-1.671445
H	-5.173031	-2.042243	-0.176538
H	-4.441763	-1.210582	2.274645
H	-1.765547	-0.950746	2.313548
H	-2.317922	0.919446	-2.509163
H	-4.932227	1.069266	-1.894323
H	-5.150693	1.864292	0.666094
H	-2.684216	2.192018	1.662428
H	4.911280	-0.087373	2.211329

H	5.140063	0.196447	-2.049543
H	3.284726	0.282487	-3.389119
H	1.915874	-0.677349	-2.826087
H	1.862940	1.072341	-2.703078
H	2.302404	0.896537	3.001741
H	1.217202	-0.339016	2.370231
H	2.714121	-0.799309	3.188252
H	7.147796	-0.675114	-0.500496
H	7.105341	1.047822	-0.143808
H	7.066589	-0.123058	1.177869
H	1.264468	-4.538423	1.513711
H	1.545232	-2.822717	1.822346
H	-0.097039	-3.492652	1.919776
H	2.434170	-4.331494	-0.744884
H	1.892659	-3.154542	-1.940507
H	2.724662	-2.611849	-0.471780
H	0.163088	-5.327472	-0.590696
H	-1.262460	-4.355944	-0.226941
H	-0.449885	-4.195238	-1.796992
H	0.673996	4.520266	1.963773
H	-0.754557	3.490718	2.015092
H	0.852279	2.794685	2.297893
H	0.015279	5.339066	-0.333554
H	-0.226437	4.218082	-1.676243
H	-1.413406	4.303434	-0.363397
H	2.292204	4.427386	0.055193
H	2.583824	2.713053	0.362998
H	2.118505	3.258635	-1.255069

$TS_{invers3+}$

E(B3LYP/6-31G*)= -3022.1462486

C	-3.169500	0.013536	-1.200821
C	-2.322710	0.012745	-0.061226
C	-2.915762	0.042424	1.225280
C	-4.309746	0.034328	1.348685
C	-5.151667	0.015166	0.234481
C	-4.556230	0.016723	-1.031661
B	-0.756266	-0.019321	-0.221426
P	0.142801	1.586769	-0.185235
C	-0.489174	3.365882	0.064687
C	-2.023047	3.371834	-0.061463
C	-2.086021	0.140432	2.490120
C	-6.652691	-0.027585	0.388021
C	-2.605651	0.026644	-2.606250
C	1.957851	1.624989	-0.361063
C	2.927084	1.909913	0.667357
C	4.235105	1.700516	0.135944
C	4.090614	1.283090	-1.221120
C	2.703356	1.255198	-1.527132
Fe	3.119551	-0.063255	0.089375
C	4.106008	-1.945242	0.404066
C	3.052024	-2.043742	-0.543454
C	1.814943	-1.638537	0.076329
C	2.157296	-1.291466	1.436291
C	3.554187	-1.476964	1.626114
P	0.186863	-1.629048	-0.807715

C	-0.628967	-3.245109	-0.150386
C	-0.938121	-3.252707	1.353051
C	0.345917	-4.391974	-0.487080
C	-1.927672	-3.445332	-0.956943
C	0.125323	4.243510	-1.044179
C	-0.073387	3.899324	1.449014
H	2.693648	2.209508	1.680444
H	1.464346	-0.917939	2.178811
H	4.108437	-1.266987	2.532918
H	5.154137	-2.144721	0.217540
H	3.155183	-2.350032	-1.576963
H	5.170537	1.836410	0.663602
H	4.894806	1.020928	-1.897281
H	2.265562	0.933732	-2.464045
H	-5.191725	0.020635	-1.914859
H	-4.748626	0.049440	2.344333
H	-2.658640	-0.189794	3.362421
H	-1.173814	-0.463522	2.442538
H	-1.771304	1.174847	2.683119
H	-2.041881	-0.886394	-2.832842
H	-3.405647	0.109562	-3.347627
H	-1.918203	0.867643	-2.760755
H	-7.154555	0.510761	-0.422615
H	-7.020215	-1.062022	0.365485
H	-6.972407	0.410730	1.338613
H	-1.342313	-4.233157	1.637834
H	-0.041741	-3.086421	1.961791
H	-1.687314	-2.501519	1.612988
H	-2.375961	-4.407159	-0.677524
H	-2.664445	-2.664246	-0.752892
H	-1.734022	-3.471122	-2.034955
H	-0.133886	-5.349498	-0.249783
H	0.608904	-4.408308	-1.550743
H	1.270524	-4.339246	0.098456
H	-0.223335	5.275714	-0.914979
H	1.219981	4.261119	-1.001637
H	-0.177390	3.906828	-2.040485
H	-0.458145	4.919659	1.572266
H	-0.479129	3.286918	2.259954
H	1.015078	3.950923	1.561420
H	-2.366737	4.409377	0.032072
H	-2.358886	2.992038	-1.030313
H	-2.508957	2.785165	0.721347

$(FeCp(C_5H_4))_2PPh^+$

E(B3LYP/6-31G*)= -3872.998984

C	0.717019	2.808861	0.958959
C	0.696216	2.130862	-0.272393
C	1.274892	2.743060	-1.395531
C	1.880017	3.996888	-1.287376
C	1.901363	4.657532	-0.058378
C	1.315854	4.063960	1.063325
P	-0.047686	0.462490	-0.518659
C	0.944875	-0.702253	0.461768
C	1.746192	-0.495534	1.640421
C	2.298127	-1.749445	2.028643

C	1.856379	-2.741913	1.103498
C	1.031071	-2.105732	0.133015
Fe	2.882166	-1.253186	0.117503
C	4.748764	-1.982095	-0.362064
C	3.933849	-1.910511	-1.530173
C	3.535491	-0.553113	-1.705332
C	4.103543	0.216170	-0.644339
C	4.855276	-0.668570	0.183013
C	-1.546669	0.623248	0.556320
C	-2.002945	-0.294070	1.551786
C	-3.277330	0.135771	2.035151
C	-3.636050	1.318861	1.319295
C	-2.585620	1.596261	0.392626
Fe	-3.462356	-0.276068	0.028248
C	-4.666172	-1.943587	-0.215362
C	-5.363951	-0.803672	-0.716857
C	-4.604100	-0.259761	-1.790522
C	-3.440109	-1.053514	-1.957511
C	-3.469154	-2.094901	-0.985070
H	1.918944	0.452388	2.131001
H	2.964418	-1.914076	2.865539
H	2.127795	-3.789379	1.117739
H	0.562930	-2.584039	-0.718400
H	3.976257	1.279255	-0.490346
H	5.395882	-0.395543	1.079906
H	5.193628	-2.879068	0.048672
H	3.655232	-2.742879	-2.163188
H	-1.459743	-1.171077	1.879979
H	-3.858060	-0.345660	2.811649
H	-4.539511	1.900524	1.451479
H	-2.564392	2.419305	-0.310977
H	-2.719689	-2.864515	-0.854764
H	-4.990673	-2.585005	0.593480
H	-6.299910	-0.411745	-0.339973
H	-4.850695	0.630758	-2.354870
H	-2.639012	-0.865911	-2.661346
H	2.906426	-0.175584	-2.500841
H	1.250848	2.238175	-2.357820
H	2.326958	4.458118	-2.163305
H	2.368030	5.634673	0.025812
H	1.327473	4.578566	2.020004
H	0.266127	2.359163	1.839471

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