Electronic Supplementary Material (ESI) for ChemComm.

Electronic Supporting Information

Lewis Acid-Base Interactions between Platinum(II) Diaryl Complexes and Bis(perfluorophenyl)zinc: Strongly Accelerated Reductive Elimination Induced by a Z-Type Ligand

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General Considerations

Unless otherwise noted, all experiments were conducted using standard Schlenk techniques or in a nitrogen atmosphere glovebox. Solvents were stored over 3 Å molecular sieves after drying with a JC Meyers Phoenix SDS solvent purification system. Deuterated solvents were purchased from Cambridge Isotope Laboratories and were degassed and dried using appropriate drying agents prior to use. $Pt(SEt_2)_2$(4-*tert*-butylphenyl)$_2$ was prepared by a method analogous to that of van Koten and coworkers,[1] and $Zn(C_6F_5)_2(\eta^2$-toluene) was prepared according to a literature procedure.[2] The ligands 1,10-phenanthroline, 2,2′-bipyridyl, and bis(dimethylphosphino)ethane were purchased from Aldrich and used as received.

Solution NMR spectroscopy was performed using Bruker NMR spectrometers at 20 ^oC unless otherwise noted. ^1H NMR spectra were calibrated internally to the residual proteo solvent relative to tetramethylsilane,[3] ^{19}F NMR chemical shifts are referenced to 1,3,5-tris(trifluoromethyl)benzene (δ –63.17 ppm vs. $CFCl_3$ in C_6D_6 at 24 °C), ^{31}P NMR chemical shifts are reported relative to H_3PO_4, and ^{195}Pt NMR chemical shifts are referenced to K_2PtCl_4 in D_2O. Elemental analyses were performed by the University of California, Berkeley College of Chemistry Microanalytical Facility. For elemental analysis results of samples containing solvent molecules, the percentage of solvent was confirmed by ^1H NMR spectroscopy.

Single crystal X-ray diffraction was performed at the UC Berkeley CheXray crystallographic facility. Measurements were performed on a Bruker AXS diffractometer with a goniostat coupled to an APEX-II CCD area detector with Mo Kα radiation (λ = 0.71073 Å) monochromated by QUAZAR multilayer mirrors. Crystals were maintained at 100(2) K during collection. Data collection, refinement, and reduction were performed with Bruker APEX2 software (v. 2014.11-0). Structures were solved with SHELXT-2014 software[4] and refined with SHELXL-2014 software[5] with refinement of F^2 against all reflections by full-matrix least squares. Non-hydrogen atoms were refined anisotropically, and hydrogen atoms were included at geometrically-calculated positions and refined using a riding model.

DFT calculations were carried out using the QChem 4.3 software package.[6] All geometries were minimized and EDA and COVPs were calculated with the B3LYP-D3 functional.[7] Light atoms (C, H, N, P, F, Zn) employed the 6-31G* basis set while Pt was treated with the SRSC ECP pseudopotential.[8] COVP images were generated with the IQmol visualization software.

Synthesis of (phen)Pt(4-^{t}Bu-Ph)$_2$ (1).

A solution of $Pt(SEt_2)_2$(4-*tert*-butylphenyl)$_2$ (116 mg, 0.180 mmol) in 8 mL of benzene was added to a stirred suspension of 1,10-phenanthroline (32.0 mg, 0.180 mmol) in 2 mL of benzene under air. After 16 hours, volatile components were removed under reduced pressure. Following trituration with pentane (3 x 5 mL), (phen)Pt(4-^{t}Bu-Ph)$_2$ (**1**) was isolated as a yellow powder (92.0 mg, 80% yield). ^1H NMR (C_6D_6, 600.13 MHz) δ 9.00 (d, J = 5.0 Hz, 2H, phen H2 and H9), 8.19 (d with Pt satellites, J_{PtH} = 69 Hz, J_{HH} = 7.8 Hz, 4H, *o*-Ar), 7.46 (d, J = 7.7 Hz, 4H, *m*-Ar), 7.21 (d, J = 8.2 Hz, 2H, phen H4 and H7), 6.82 (s, 2H, phen H5 and H6), 6.37 (dd, J = 8.2, 5.0 Hz, 2H, phen H3 and H8); 1.42 (s, 18H, ^{t}Bu); ^1H NMR (CD_2Cl_2, 600.13 MHz) δ 8.80 (d, J = 5.0 Hz, 2H, phen H2 and H9), 8.58 (d, J = 8.2 Hz, 2H, phen H4 and H7), 7.97 (s, 2H, phen H5 and H6), 7.74 (dd, J = 8.2, 5.0 Hz, 2H, phen H3 and H8), 7.46 (d with Pt satellites, J_{PtH} = 67 Hz,

J_{HH} = 7.8 Hz, 4H, *o*-Ar), 7.11 (d, *J* = 7.8 Hz, 4H, *m*-Ar), 1.33 (s, 18H, ^{t}Bu); $^{13}C\{^{1}H\}$ NMR (CD_2Cl_2, 150.9 MHz) δ 150.38 (phen C2 and C9), 148.06 (phen), 144.65 (*ipso*-Ar), 141.50 (*p*-Ar), 138.15 (*o*-Ar), 137.16 (phen C4 and C7), 130.84 (phen), 127.76 (phen H5 and H6), 126.23 (phen H3 and H8), 124.50 (*m*-Ar), 34.35 (–*C*(CH_3)$_3$), 31.96 (–C(*C*H_3)$_3$); $^{195}Pt\{^{1}H\}$ NMR (CD_2Cl_2, 129 MHz) δ –3355. Anal. Calc. for $C_{32}H_{34}N_2Pt$•0.67C_6H_6 (%) C 62.32, H 5.52, N 4.04; Found C 62.57, H 5.15, N 3.85.

Synthesis of (phen)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (2).

A solution of **1** (9.6 mg, 0.015 mmol) and Zn(C_6F_5)$_2$(η^2-toluene) (7.5 mg, 0.015 mmol) was prepared in 0.5 mL of toluene. The solution was filtered, and vapor diffusion of pentane into the toluene solution at –35 °C afforded yellow crystals of (phen)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (**2**, 9.5 mg, 56% yield). ^{1}H NMR (C_6D_6, 600.13 MHz) δ 8.93 (d, *J* = 5.0 Hz, 2H, phen H2 and H9), 7.67 (d with Pt satellites, J_{PtH} = 50 Hz, J_{HH} = 7.8 Hz, 4H, *o*-Ar), 7.30 (d, *J* = 8.1 Hz, 4H, *m*-Ar), 7.19 (d, *J* = 8.2 Hz, 2H, phen H4 and H7), 6.89 (s, 2H, phen H5 and H6), 6.51 (dd, *J* = 8.1, 5.0 Hz, 2H, phen H3 and H8), 1.33 (s, 18H, ^{t}Bu); $^{13}C\{^{1}H\}$ NMR (C_6D_6, 150.9 MHz) δ 151.60 (phen 2 and 9), 147.70 (phen), 147.05 (*ipso*-Ar), 138.66 (*o*-Ar), 138.23 (phen), 137.93 (phen C4 and C7), 136.09 (*p*-Ar), 127.19 (phen C5 and C6), 126.03 (*m*-Ar), 125.57 (phen C3 and C8), 34.65 (–*C*(CH_3)$_3$), 32.03 (–C(*C*H_3)$_3$); C_6F_5 resonances not observed; ^{19}F NMR (C_6D_6, 376 MHz) δ –116.97, –156.23, –160.81; $^{195}Pt\{^{1}H\}$ NMR (C_6D_6, 129 MHz) δ –3167. Anal. Calc. for $C_{44}H_{34}N_2PtZn$•0.5C_7H_8 (%) C 52.47, H 3.52, N 2.58; Found C 52.27, H 3.56, N 2.75.

Synthesis of (bpy)Pt(4-^{t}Bu-Ph)$_2$ (3).

A solution of Pt(SEt_2)$_2$(4-*tert*-butylbenzene)$_2$ (116 mg, 0.180 mmol) in 8 mL of benzene was added to a stirred suspension of 2,2′-bipyridyl (28.0 mg, 0.180 mmol) in 2 mL of benzene under air. After 16 hours, volatile components were removed under reduced pressure. Following trituration with pentane (3 x 5 mL), yellow crystals of (bpy)Pt(4-^{t}Bu-Ph)$_2$ (**3**) were isolated by recrystallization from a toluene/hexanes solution at –30 °C (87.1 mg, 73% yield).^{1}H NMR (CD_2Cl_2, 600.13 MHz) δ 8.49 (dt, *J* = 5.3, 1.2 Hz, 2H, bpy H6), 8.15 – 8.04 (m, 4H, bpy H3 and H4), 7.41 (td, *J* = 5.8, 2.7 Hz, 2H, bpy H5), 7.36 (d with Pt satellites, J_{PtH} = 60 Hz, J_{HH} = 6.0 Hz, 4H, *o*-Ar), 7.06 (d, *J* = 6.0 Hz, 4H, *m*-Ar), 1.30 (s, 18H, ^{t}Bu); $^{13}C\{^{1}H\}$ NMR (CD_2Cl_2, 150.9 MHz) δ 156.61 (bpy C2, 150.35 (bpy C6), 144.55 (*ipso*-Ar), 142.09 (*p*-Ar), 137.86 (*o*-Ar and bpy C4), 127.55 (bpy C5), 124.50 (*m*-Ar), 122.80 (bpy C3), 34.31 (–*C*(CH_3)$_3$), 31.92 (–C(*C*H_3)$_3$); $^{195}Pt\{^{1}H\}$ NMR (CD_2Cl_2, 129 MHz) δ –3328. Anal. Calc. for $C_{30}H_{34}N_2Pt$·0.33C_7H_8 (%) C59.89, H 5.70, N 4.32; Found C 59.56, H 5.70, N 4.32.

Synthesis of (bpy)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (4).

A solution of **2** (11 mg, 0.017 mmol) and Zn(C_6F_5)$_2$(η^2-toluene) (9.2 mg, 0.019 mmol) was prepared in 0.5 mL of toluene. The solution was filtered, and vapor diffusion of pentane into the toluene solution at –35 °C afforded yellow crystals of (bpy)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (**4**, 11 mg, 64% yield). ^{1}H NMR (C_6D_6, 600.13 MHz) δ 8.60 (d, *J* = 5.5 Hz, 2H, bpy H6), 7.59 (d with Pt satellites, J_{PtH} = 42 Hz, J_{HH} = 7.8 Hz, 4H, *o*-Ar), 7.25 (d, *J* = 7.8 Hz, 4H, *m*-Ar), 6.74 (t, *J* = 7.8

Hz, 2H, bpy H4), 6.60 (d, J = 8.1 Hz, 2H, bpy H3), 6.18 (t, J = 6.6 Hz, 2H, bpy H5), 1.26 (s, 18H, ^{t}Bu); $^{13}C\{^1H\}$ NMR (CD_2Cl_2, 150.9 MHz) δ 155.94 (bpy C2), 151.22 (bpy C6), 147.79 (*ipso*-Ar), 138.23 (*o*-Ar), 138.11 (bpy C4), 136.01 (*p*-Ar), 126.85 (bpy C5), 126.02 (*m*-Ar), 122.15 (bpy C3), 34.59 (–*C*(CH_3)$_3$), 31.93 (–C(*C*H_3)$_3$); ^{19}F NMR (376 MHz, C_6D_6) δ –116.53, –156.16, –160.76; $^{195}Pt\{^1H\}$ NMR (C_6D_6, 129 MHz) δ –3150. Anal. Calc. for $C_{42}H_{34}F_{10}N_2PtZn$ (%) C 49.59, H 3.37, N 2.75; Found C 49.44, H 3.23, N, 3.10.

Synthesis of (dmpe)Pt(4-^{t}Bu-Ph)$_2$ (5).

Bis(dimethylphosphino)ethane (30.0 μL, 0.180 mmol) was added to a stirred solution of $Pt(SEt_2)_2$(4-*tert*-butylbenzene)$_2$ (116 mg, 0.180 mmol) in 8 mL of toluene. After 20 minutes, volatile components were removed under reduced pressure, and the resulting white powder was triturated with hexanes (3 x 4 mL) to afford (dmpe)Pt(4-^{t}Bu-Ph)$_2$ (**5**, 93.6 mg, 85% yield). ^1H NMR (C_6D_6, 600.13 MHz) δ 7.85 (dd with Pt satellites, J_{PtH} = 57 Hz, J_{HH} = 5.0 Hz, J_{PH} = 7.0 Hz, 4H, *o*-Ar), 7.33 (d, J_{HH} = 5.0 Hz, 4H, *m*-Ar), 1.28 (s, 18H, ^{t}Bu), 0.95 – 0.74 (m, 16H, dmpe); $^{13}C\{^1H\}$ NMR (C_6D_6, 150.9 MHz) δ 159.45 (*ipso*-Ar), 144.12 (*p*-Ar), 137.42 (J_{PtH} = 37 Hz, *o*-Ar), 125.01 (J_{PtH} = 63 Hz, *m*-Ar), 34.40 (–*C*(CH_3)$_3$), 32.24 (–C(*C*H_3)$_3$), 29.38 (br, dmpe), 11.96 (d, J_{PH} = 27 Hz, dmpe); ^{31}P NMR (C_6D_6) δ 21.23 (s with Pt satellites, J_{PtP} = 1630.5 Hz); $^{195}Pt\{^1H\}$ NMR (C_6D_6, 129 MHz) δ –4506 (t, J_{PtP} = 1631.0 Hz). Anal. Calc. for $C_{26}H_{42}P_2Pt$ (%) C 51.06, H 6.92; Found C 50.99, H 6.74.

Synthesis of (dmpe)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (6).

A solution of **5** (10. mg, 0.016 mmol) and Zn(C_6F_5)$_2$(η^2-toluene) (8.1 mg, 0.016 mmol) was prepared in 0.5 mL of toluene. The solution was filtered, and vapor diffusion of pentane into the toluene solution at –35 °C afforded colorless crystals of (dmpe)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (**6**, 11 mg, 68% yield). ^1H NMR (C_6D_6, 600.13 MHz) δ 8.03 (dd with Pt satellites, J_{PtH} = 42.0 Hz, J_{PH} = 7.9 Hz, J_{HH} = 6.0 Hz, 4 H, *o*-Ar), 7.36 (d, J_{HH} = 6.0 Hz, 4H, *m*-Ar), 1.23 (s, 18H, ^{t}BuAr), 0.64 (m, 4H, dmpe), 0.55 (m, 12H, dmpe); $^{13}C\{^1H\}$ NMR (C_6D_6, 150.9 MHz) δ 151.56 (*p*-Ar), 141.69 (J_{PtH} = 24 Hz, *o*-Ar), 127.51 (J_{PtH} = 45 Hz, *m*-Ar), 34.66 (–*C*(CH_3)$_3$), 31.64 (–C(*C*H_3)$_3$), 27.89 (br, dmpe), 10.90 (d, J_{PH} = 32 Hz, dmpe), *ipso*-carbon and Zn-Ar^F groups not observed; ^{31}P NMR (C_6D_6) δ 29.37 (s with Pt satellites, J_{PtP} = 2142.3 Hz); ^{19}F NMR (C_6D_6, 376 MHz) δ –111.77, –147.84, –155.07; $^{195}Pt\{^1H\}$ NMR (C_6D_6, 129 MHz) δ –4544 (t, J_{PtP} = 2138.8 Hz). Anal. Calc. for $C_{38}H_{42}F_{10}P_2PtZn$ (%) C 45.14, H 4.19; Found C 44.76, H 4.50.

Attempted thermolysis of (phen)Pt(4-^{t}Bu-Ph)$_2$ (1).

A solution of **1** (3.2 mg, 0.0050 mmol) was prepared in 0.500 mL of mesitylene-d_{12} in a J. Young NMR tube. The NMR tube was heated to 200 ^{o}C in a temperature-controlled oil bath. No reaction was observed by ^1H NMR spectroscopy after 48 hours.

Biaryl reductive elimination from (phen)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (2).

A solution of **1** (3.2 mg, 0.0050 mmol), Zn(C_6F_5)$_2$(η^2-toluene) (25 mg, 0.050 mmol), and ferrocene as an internal standard was prepared in 0.5 mL of benzene-d_6. The sample was stored at 0 °C prior to insertion into an NMR spectrometer with a sample temperature pre-equilibrated to 60 °C. Complete conversion to 4,4′-di-*tert*-butylbiphenyl[9] and (phen)Zn(C_6F_5)$_2$[10] was observed by ^{1}H and ^{19}F NMR spectroscopy within 15 minutes. ^{1}H NMR of 4,4′-di-*tert*-butylbiphenyl: δ 7.58 (d, *J* = 8.2 Hz, 4H), 7.37 (d, *J* = 8.1 Hz, 4H), 1.28 (s, 18H); ^{1}H NMR of (phen)Zn(C_6F_5)$_2$: δ 9.05 (d, *J* = 4.4 Hz, 2H), 7.22 (dd, *J* = 8.2, 1.4 Hz, 2H), 6.86 (s, 2H), 6.75 (dd, *J* = 8.2, 4.8 Hz, 2H); ^{19}F NMR of (phen)Zn(C_6F_5)$_2$: δ –116.04, –156.84, –161.01.

Biaryl reductive elimination from (phen)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (2) in the presence of tri-*tert*-butylphosphine.

A solution of **1** (3.2 mg, 0.0050 mmol), Zn(C_6F_5)$_2$(η^2-toluene) (25 mg, 0.050 mmol), and tri-*tert*-butylphosphine (10. mg, 0.050 mmol) was prepared in 0.5 mL of benzene-d_6 in a J. Young NMR tube. After heating the NMR tube to 60 °C for 24 hours in a temperature-controlled oil bath, complete conversion to 4,4′-di-*tert*-butylbiphenyl, (phen)Zn(C_6F_5)$_2$, and Pt(P^{t}Bu$_3$)$_2$[11] was observed by ^{1}H, ^{19}F, and ^{31}P NMR spectroscopy.

Biaryl reductive elimination from (bpy)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (4).

A solution of **3** (3.1 mg, 0.0050 mmol) and Zn(C_6F_5)$_2$(η^2-toluene) (25 mg, 0.050 mmol) was prepared in 0.5 mL of benzene-d_6 in a J. Young NMR tube. The NMR tube was heated to 60 °C in a temperature-controlled oil bath. Complete conversion to 4,4′-di-*tert*-butylbiphenyl and (bpy)Zn(C_6F_5)$_2$[12] was observed by ^{1}H and ^{19}F NMR spectroscopy within 15 minutes. ^{1}H NMR of (bpy)Zn(C_6F_5)$_2$: δ 8.87 (d, *J* = 5.0 Hz, 2H), 6.87 (m, 4H), 6.65 (m, 2H).

Attempted thermolysis of (dmpe)Pt(4-^{t}Bu-Ph)$_2$ (5).

A solution of **5** (3.1 mg, 0.0050 mmol) was prepared in 0.5 mL of toluene-d_8 in a J. Young NMR tube. The NMR tube was heated to 60 °C in a temperature-controlled oil bath. No reaction was observed by ^{1}H or ^{31}P NMR spectroscopy after 24 hours.

Thermolysis of (dmpe)Pt(4-^{t}Bu-Ph)$_2$[Zn(C_6F_5)$_2$] (6).

A solution of **5** (3.1 mg, 0.0050 mmol) and Zn(C_6F_5)$_2$(η^2-toluene) (25.0 mg, 0.0500 mmol) was prepared in 0.5 mL of toluene-d_8 in a J. Young NMR tube. The NMR tube was heated to 60 °C in a temperature-controlled oil bath. After 65 hours, complete conversion to (dmpe)Pt(C_6F_5)$_2$[13] and bis(4-*tert*-buylphenyl)zinc[14] was observed by ^{1}H, ^{19}F, and ^{31}P NMR spectroscopy. ^{1}H NMR of bis(4-*tert*-butylphenyl)zinc: δ 7.56 (d, *J* = 7.7 Hz, 4H), 7.53 (d, *J* = 7.7 Hz, 4H), 1.46 (s, 18H);

^{19}F NMR of (dmpe)Pt(C_6F_5)$_2$: δ –118.9 (m with Pt satellites, J_{PtF} = 330 Hz, 4F),–162.1 (m, 2F), –163.2 (m, 4F); ^{31}P NMR of (dmpe)Pt(C_6F_5)$_2$: δ 26.5 (br m, J_{PtP} = 2245 Hz).

Table S1. Crystal data and structure refinement for **2**.

Empirical formula	C51 H42 F10 N2 Pt Zn	
Formula weight	1133.32	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/c	
Unit cell dimensions	a = 12.9950(13) Å	α= 90°
	b = 16.7483(16) Å	β= 106.136(2)°
	c = 21.185(2) Å	γ = 90°
Volume	4429.1(7) $Å^3$	
Z	4	
Density (calculated)	1.700 Mg/m^3	
Absorption coefficient	3.777 mm^{-1}	
F(000)	2240	
Crystal size	0.120 x 0.100 x 0.040 mm^3	
Theta range for data collection	1.575 to 25.373°	
Index ranges	–15<=h<=15, –20<=k<=20, –25<=l<=25	
Reflections collected	90981	
Independent reflections	8095 [R(int) = 0.0344]	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.3529 and 0.2655	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8095 / 0 / 593	
Goodness-of-fit on F^2	1.156	
Final R indices [I>2sigma(I)]	R1 = 0.0312, wR2 = 0.0722	
R indices (all data)	R1 = 0.0355, wR2 = 0.0747	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.648 and –0.649 $e/Å^3$	

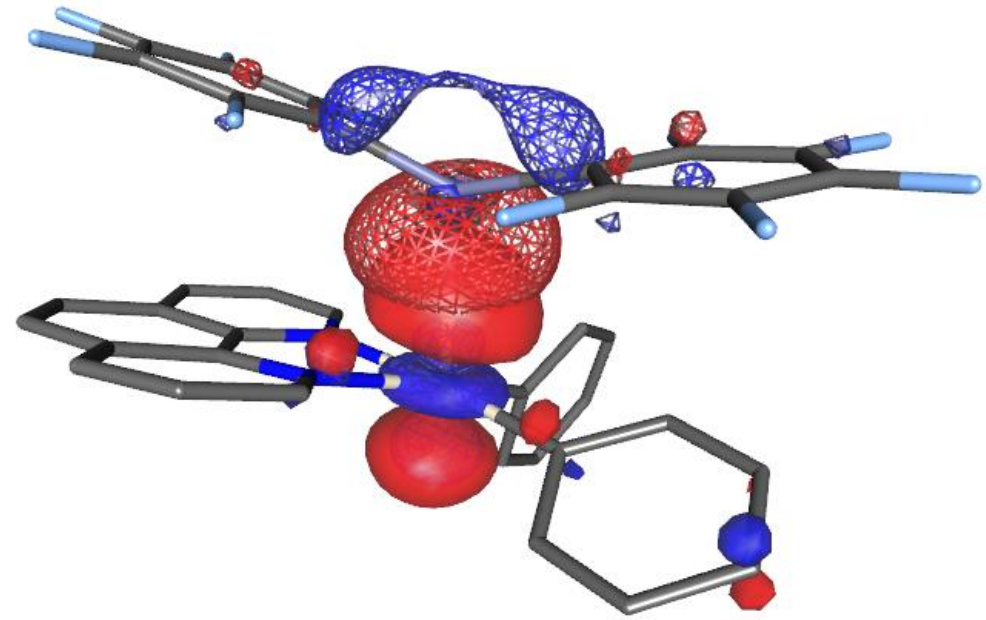
Table S2. Crystal data and structure refinement for **6**.

Empirical formula	C38 H42 F10 P2 Pt Zn	
Formula weight	1011.11	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 2_1/n	
Unit cell dimensions	a = 10.9506(3) Å	α= 90°
	b = 19.9969(6) Å	β= 96.0540(10)°
	c = 17.6775(6) Å	γ = 90°
Volume	3849.4(2) $Å^3$	
Z	4	
Density (calculated)	1.745 Mg/m^3	
Absorption coefficient	4.412 mm^{-1}	
F(000)	1992	
Crystal size	0.120 x 0.100 x 0.070 mm^3	
Theta range for data collection	1.542 to 25.358°	
Index ranges	–13<=h<=13, 0<=k<=23, 0<=l<=21	
Reflections collected	7042	
Independent reflections	7042	
Completeness to theta = 25.000°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.303439 and 0.250108	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7042 / 0 / 558	
Goodness-of-fit on F^2	1.206	
Final R indices [I>2sigma(I)]	R1 = 0.0252, wR2 = 0.0560	
R indices (all data)	R1 = 0.0315, wR2 = 0.0622	
Extinction coefficient	n/a	
Largest diff. peak and hole	0.823 and –1.459 e/$Å^3$	

DFT Results

(phen)PtAr$_2$(ZnAr$^F_2$) (2)

d(Pt)→p(Zn)



d(Zn)→σ*(PtAr)

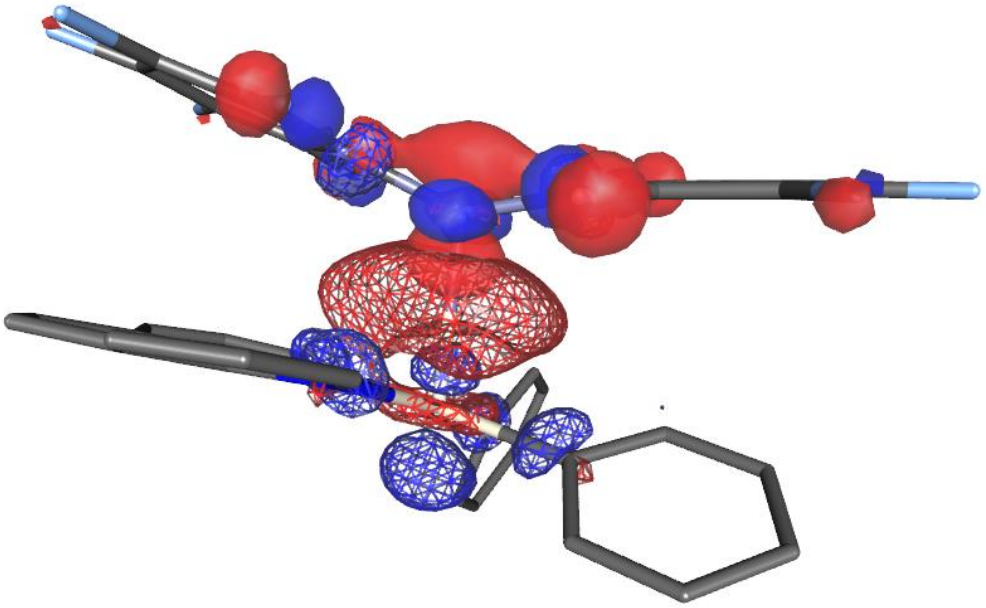


Figure S1. Selected COVPs for **2**. Occupied orbitals are represented by solid intense colors, and complementary virtual orbitals have mesh isosurfaces. Hydrogen atoms and ^{t}Bu are omitted for clarity.

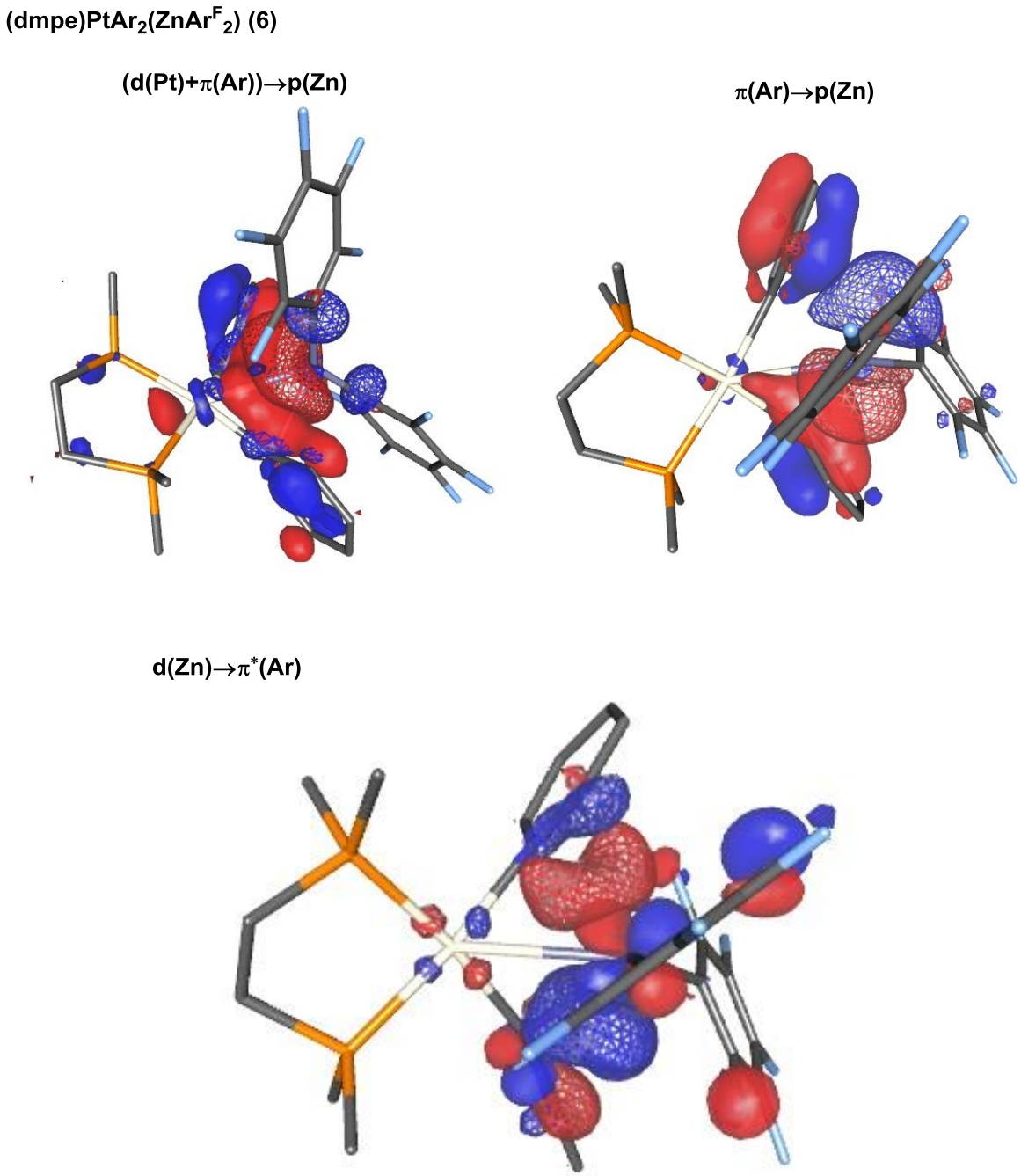


Figure S2. Selected COVPs for **6**. Occupied orbitals are represented by solid intense colors, and complementary virtual orbitals have mesh isosurfaces. Hydrogen atoms and ^{t}Bu are omitted for clarity.

(dmpe)PtAr$_2$(ZnAr$^F_2$) (basal Zn location)

```
Fragment 1 coords
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C   -1.0578096609   1.520223361   -0.6951937631
C   -0.5971658161   1.9588010909   -1.9534477964
H   -0.5055531815   1.2463264283   -2.7685320947
C   -0.2439300378   3.2764619317   -2.1952682541
H   0.1185995791   3.5402762849   -3.1850033954
C   -0.2830615814   4.249468617   -1.1832934586
C   -0.7716899126   3.8430003035   0.0608019329
H   -0.8429829994   4.5461039281   0.8832449218
C   -1.1705560003   2.5184721594   0.2923565027
H   -1.5753031716   2.2667632012   1.2666352407
C   0.2437140311   5.6572029282   -1.479728346
C   0.1484737001   -1.376884614   -0.7495433218
C   0.8975363845   -1.2811195826   -1.9389880746
H   0.628396955   -0.5369918317   -2.682240694
C   1.9776293312   -2.116211492   -2.2002287196
H   2.4950534136   -2.0112666039   -3.1495550439
C   2.3980507031   -3.0924412943   -1.277983249
C   1.6888885619   -3.1621204647   -0.0741274467
H   1.9838107739   -3.8667383714   0.6948784011
C   0.5911570779   -2.3352032882   0.1802737324
H   0.0749384643   -2.4426408929   1.1277503092
C   3.5096371662   -4.0890672714   -1.6409209616
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The format for covp energy -> orb_index printing is as follows:
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(charge_contribution[mili e-]) (donor_orb_index) (acceptor_orb_index)
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this is how $plots indexes
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Charge Transfer Calculation Completed
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E(Pfrz) = -5053.0539009658
E(scf) = 9999.9000000000
dE(non-frz) / kJ/mol = 39521999.4939381480
Fragment Energies (Ha)
  -1.8183e+03
  -3.2347e+03
PRINTING EDA DATA in kJ/mol:
E_frz = 6.1205415475
E_pol = -135.2166372083
E_pct = -172.3678692844
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(phen)PtAr$_2$(ZnAr$^F{}_2$) (apical Zn location)

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H   3.0666610565   -1.5771631129   0.1568880154
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C	0.7011610609	-4.2155612227	1.6571825307
C	-0.2755099826	-5.1292513615	2.1749142451
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H	-4.5237661222	-1.1548821534	2.502943679
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C	0.3694117981	-2.8468294652	1.5297554707
C	2.2728386268	0.8351824347	0.5405451093
C	2.7135413448	1.1937640909	-0.738097798
H	2.0113394827	1.2417616349	-1.5655326192
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H	4.3421129194	1.7478046298	-2.0008548884
C	5.0252420375	1.4382484674	0.0261879218
C	4.5740902466	1.1060139945	1.3141991258
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Fragment 2 coords
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Fragment 1 energy: -1468.9495449568
Fragment 2 energy: -3234.7179315819

Row To Col CT Energy kJ/mol
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  -9.9232e+01   1.8550e-06
Row To Col CT Charge me-
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The format for covp energy -> orb_index printing is as follows:
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(spin)  (d+1) (a+1) (energy_contribution[kj/mol])
(charge_contribution[mili e-]) (donor_orb_index) (acceptor_orb_index)
Fragment indices printed here start at 1 and so do orbital indices as
this is how $plots indexes
Totals (energy and charge) for each d,a pair should have already been
printed above
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Charge Transfer Calculation Completed
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Sum of fragment energies:    -4703.6674765387
E(Pfrz) = -4703.6903024682
E(scf) = 9999.9000000000
dE(non-frz) / kJ/mol = 38604734.4804486707
Fragment Energies (Ha)
  -1.4689e+03
  -3.2347e+03
PRINTING EDA DATA in kJ/mol:
E_frz = -59.9301889321
E_pol = -81.2199805314
E_pct = -139.5144817000
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(dmpe)PtAr$_2$(ZnAr$^F_2$) (apical Zn location)

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C          2.64737       -3.01787        0.31870
H          2.35902       -2.86696       -0.71951
C         -3.29735       -1.04746        1.94646
H         -3.48417        0.01123        2.13511
C         -1.36573       -3.25561        1.96319
C          0.01588       -3.74421        1.44869
C          2.20816        0.44762        0.70798
C          2.72066        0.21016       -0.57282
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H	2.15027	-0.37326	-1.28919
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H	2.66646	1.41679	2.58652
C	6.16498	1.95959	-0.49788
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H	6.56443	0.55443	-2.13895
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C	6.17799	3.49635	-0.33244
H	5.41909	3.96083	-0.97234
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P	-1.52120	-1.40208	2.25792
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Fragment 2 coords
0 1
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C         -0.69664       -4.97365       -2.43715
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F         -2.78367       -2.50502       -0.82062
F          0.34887        1.76202       -3.13108
F         -0.67144        4.19840       -3.79305
F         -2.99610        5.05060       -2.64871
F         -4.29526        3.47919       -0.83402
F         -3.28607        1.04074       -0.18735
Zn        -0.64712       -0.36068       -1.07778

Fragment 1 energy: -1818.3431810084
Fragment 2 energy: -3234.7157588006

Row To Col CT Energy kJ/mol
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  -1.1214e+02  -5.1301e-07
Row To Col CT Charge me-
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   59.1535   -1.8771

The format for covp energy -> orb_index printing is as follows:
(spin)  (d+1) (a+1) (energy_contribution[kj/mol])
(charge_contribution[mili e-]) (donor_orb_index) (acceptor_orb_index)
Fragment indices printed here start at 1 and so do orbital indices as
this is how $plots indexes
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Totals (energy and charge) for each d,a pair should have already been
printed above
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Charge Transfer Calculation Completed
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Sum of fragment energies:    -5053.0589398090
E(Pfrz) = -5053.0760611879
E(scf) = 9999.9000000000
dE(non-frz) / kJ/mol = 39522057.6762916222
Fragment Energies (Ha)
  -1.8183e+03
  -3.2347e+03
PRINTING EDA DATA in kJ/mol:
E_frz = -44.9527138719
E_pol = -95.6008078120
E_pct = -149.3329789917
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(phen)PtAr$_2$(ZnAr$^F_2$) (basal Zn position)

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C         -2.12769        2.15144       -0.08806
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Fragment 2 coords

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Fragment 1 energy: -1468.9466608298
Fragment 2 energy: -3234.7118353712

Row To Col CT Energy kJ/mol
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Row To Col CT Charge me-
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   63.0109   -1.8543

The format for covp energy -> orb_index printing is as follows:
(spin)  (d+1) (a+1) (energy_contribution[kj/mol])
(charge_contribution[mili e-]) (donor_orb_index) (acceptor_orb_index)
Fragment indices printed here start at 1 and so do orbital indices as
this is how $plots indexes
Totals (energy and charge) for each d,a pair should have already been
printed above
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Charge Transfer Calculation Completed
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Sum of fragment energies:    -4703.6584962010
E(Pfrz) = -4703.6550914627
E(scf) = 9999.9000000000
dE(non-frz) / kJ/mol = 38604642.0328568220
Fragment Energies (Ha)
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PRINTING EDA DATA in kJ/mol:
E_frz = 8.9392464325
E_pol = -99.8040392480
E_pct = -181.2641494140
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(dmpe)Pt(Ar^F)$_2$($ZnAr^F_2$)

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Fragment 1 energy: -2496.1228963287
Fragment 2 energy: -3234.7087693450
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The format for covp energy -> orb_index printing is as follows:
(spin)  (d+1) (a+1) (energy_contribution[kj/mol])
(charge_contribution[mili e-]) (donor_orb_index) (acceptor_orb_index)
Fragment indices printed here start at 1 and so do orbital indices as
this is how $plots indexes
Totals (energy and charge) for each d,a pair should have already been
printed above
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Alpha	2	1	-0.012937893468	0.001769214642	355	356
Alpha	2	1	-0.017685444296	0.001610432154	357	358
Alpha	2	1	-0.008968425512	0.001356223708	359	360
Alpha	2	1	-0.013949117232	0.000830745452	361	362
Alpha	2	1	-0.019391765100	0.000703620045	363	364
Alpha	2	1	-0.006205840101	0.000606946077	365	366
Alpha	2	1	-0.008766677984	0.000623221749	367	368
Alpha	2	1	-0.004443546114	0.000509438153	369	370
Alpha	2	1	-0.002915569916	0.000402762775	371	372
Alpha	2	1	-0.001898739650	0.000291536839	373	374
Alpha	2	1	-0.003968743440	0.000286383803	375	376
Alpha	2	1	-0.005899888820	0.000241448457	377	378
Alpha	2	1	-0.001684521144	0.000193706326	379	380
Alpha	2	1	-0.001867388031	0.000150698481	381	382
Alpha	2	1	-0.002198356208	0.000108567440	383	384
Alpha	2	1	-0.003168378748	0.000117947473	385	386
Alpha	2	1	-0.000877889037	0.000089352085	387	388

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Alpha   2   1   -0.002102900412  0.000067541041   389   390
Alpha   2   1   -0.001678056373  0.000066443947   391   392
Alpha   2   1   -0.001268238288  0.000062861370   393   394
Alpha   2   1   -0.002015065848  0.000054414679   395   396
Alpha   2   1   -0.001131288391  0.000050186254   397   398
Alpha   2   1   -0.000898890153  0.000060482081   399   400
Alpha   2   1   -0.000640102092  0.000032633514   401   402
Alpha   2   1   -0.000915901027  0.000032076385   403   404
Alpha   2   1   0.000044339749  0.000061187070   405   406
Alpha   2   1   -0.000449017417  0.000080372269   407   408
Alpha   2   1   -0.000786412309  0.000026781073   409   410
Alpha   2   1   -0.000452391312  0.000022534911   411   412
Alpha   2   1   -0.000468171802  0.000021843931   413   414
Alpha   2   1   -0.000630871279  0.000018651444   415   416
Alpha   2   1   -0.000503094504  0.000016110271   417   418
Alpha   2   1   -0.000377302268  0.000014069512   419   420
Alpha   2   1   -0.000338843315  0.000019899187   421   422
Alpha   2   1   -0.000106281980  0.000010246071   423   424
Alpha   2   1   -0.000158888688  0.000008541990   425   426
Alpha   2   1   -0.000108320592  0.000007760362   427   428
Alpha   2   1   -0.000078273673  0.000004125042   429   430
Alpha   2   1   -0.000223233092  0.000003984672   431   432
Alpha   2   1   -0.000119731559  0.000002713746   433   434
Alpha   2   1   -0.000030352587  0.000001495727   435   436
Alpha   2   1   -0.000037587541  0.000001155987   437   438
Alpha   2   1   -0.000013427908  0.000000754850   439   440
Alpha   2   1   -0.000016480405  0.000000377978   441   442
Alpha   2   1   -0.000005249471  0.000000167057   443   444
Alpha   2   1   -0.000006110838  0.000000086227   445   446
Alpha   2   1   -0.000008450093  0.000000106981   447   448
Alpha   2   1   0.000010168726  0.000000002906   449   450
Alpha   2   1   -0.000007158456  -0.000000194169   451   452
Alpha   2   1   -0.000001552066  0.000000002529   453   454

Charge Transfer Calculation Completed
=====================================================
Sum of fragment energies:    -5730.8316656738
E(Pfrz) = -5730.8146470602
E(scf) = 9999.9000000000
dE(non-frz) / kJ/mol = 41301481.4507940710
Fragment Energies (Ha)
  -2.4961e+03
  -3.2347e+03
PRINTING EDA DATA in kJ/mol:
E_frz = 44.6829001641
E_pol = -99.4801227828
E_pct = -171.0735147135
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References

1. M. A. C. Lacabra, A. J. Canty, M. Lutz, J. Patel, A. L. Spek, H. Sun and G. van Koten, *Inorg. Chim. Acta*, 2002, **327**, 15.
2. D. A. Walker, T. J. Woodman, D. L. Hughes and M. Bochmann, *Organometallics*, 2001, **20**, 3772.
3. G. R. Fulmer, A. J. M. Miller, N. H. Sherden, H. E. Gottlieb, A. Nudelman, B. M. Stoltz, J. E. Bercaw and K. I. Goldberg, *Organometallics*, 2010, **29**, 2176.
4. G. M. Sheldrick, *Acta Cryst.* 2015, **A71**, 3.
5. G. M. Sheldrick, *Acta Cryst.* 2008, **A64**, 112.
6. Y. Shao, Z. Gan, E. Epifanovsky, A. T. B. Gilbert, M. Wormit, J. Kussmann, A. W. Lange, A. Behn, J. Deng, X. Feng, D. Ghosh, M. Goldey, P. R. Horn, L. D. Jacobson, I. Kaliman, R. Z. Khaliullin, T. Kuś, A. Landau, J. Liu, E. I. Proynov, Y. M. Rhee, R. M. Richard, M. A. Rohrdanz, R. P. Steele, E. J. Sundstrom, H. L. Woodcock, P. M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire, B. Austin, G. J. O. Beran, Y. A. Bernard, E. Berquist, K. Brandhorst, K. B. Bravaya, S. T. Brown, D. Casanova, C.-M. Chang, Y. Chen, S. H. Chien, K. D. Closser, D. L. Crittenden, M. Diedenhofen, R. A. DiStasio, H. Do, A. D. Dutoi, R. G. Edgar, S. Fatehi, L. Fusti-Molnar, A. Ghysels, A. Golubeva-Zadorozhnaya, Joseph Gomes, Magnus W.D. Hanson-Heine, Philipp H.P. Harbach, Andreas W. Hauser, Edward G. Hohenstein, Z. C. Holden, T.-C. Jagau, H. Ji, B.n Kaduk, K. Khistyaev, J. Kim, J. Kim, R. A. King, P. Klunzinger, D. Kosenkov, T. Kowalczyk, C. M. Krauter, K. U. Lao, A. D. Laurent, K. V. Lawler, S. V. Levchenko, C. Y. Lin, F. Liu, E. Livshits, R. C. Lochan, A. Luenser, P. Manohar, S. F. Manzer, S.-P. Mao, N. Mardirossian, A. V. Marenich, Simon A. Maurer, Nicholas J. Mayhall, Eric Neuscamman, C. Melania Oana, Roberto Olivares-Amaya, Darragh P. O'Neill, J. A. Parkhill, T. M. Perrine, R. Peverati, A. Prociuk, D. R. Rehn, E. Rosta, N. J. Russ, S. M. Sharada, S. Sharma, D. W. Small, A. Sodt, T. Stein, D. Stück, Y.-C. Su, A. J. W. Thom, T. Tsuchimochi, V. Vanovschi, L. Vogt, O. Vydrov, T. Wang, M. A. Watson, J. Wenzel, A. White, C. F. Williams, J. Yang, S. Yeganeh, S. R. Yost, Z.-Q. You, I. Y. Zhang, X. Zhang, Y. Zhao, B. R. Brooks, G. K. L. Chan, D. M. Chipman, C. J. Cramer, W. A. Goddard, M. S. Gordon, W. J. Hehre, A. Klamt, H. F. Schaefer, M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Warshel, X. Xu, Alán Aspuru-Guzik, Roi Baer, Alexis T. Bell, Nicholas A. Besley, Jeng-Da Chai, Andreas Dreuw, Barry D. Dunietz, T. R. Furlani, S. R. Gwaltney, C.-P. Hsu, Y. Jung, J. Kong, D. S. Lambrecht, W. Liang, C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik, T. V. Voorhis, J. M. Herbert, A. I. Krylov, P. M.W. Gill and M. Head-Gordon, *Mol. Phys.*, 2015, **113**, 184.
7. R. Z. Khaliullin, A. T. Bell and M. Head-Gordon, *J. Chem. Phys.* 2008, **128**, 184112.
8. D. Andrae, U. Häußermann, M. Dolg, H. Stoll and H. Preuß, *Theor. Chim. Acta*, 1990, **77**, 123.
9. A. K. Cook and M. S. Sanford, *J. Am. Chem. Soc.*, 2015, **137**, 3109.
10. J. G. Noltes and J. W. G. van den Hurk, *J. Organomet. Chem.*, 1965, **3**, 222.

11. R. G. Goel, W. O. Ogini and R. C. Srivastava, *J. Organomet. Chem.*, 1981, **214**, 405.
12. E. Martin, C. Spendley, A. J. Mountford, S. J. Coles, P. N. Horton, D. L. Hughes, M. B. Hursthouse and S. J. Lancaster, *Organometallics*, 2008, **27**, 1436.
13. R. P. Hughes, A. J. Ward, J. A. Golden, C. D. Incarvito, A. L. Rheingold and L. N. Zahkarov, *Dalton Trans.*, **2004**, 2720.
14. L. Ilies, J. Okabe, N. Yoshikai and E. Nakamura, *Org. Lett.*, 2010, **12**, 2838.