

Supporting Information

A Rare Unsupported Iridium(II) Dimer $[\text{IrCl}_2(\text{CO})_2]_2$

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1. Experimental

1.1 General Procedures. All reactions with metal complexes were carried out under an atmosphere of purified nitrogen using standard Schlenk-vessel and vacuum line techniques. Infrared spectra were recorded in the range 4000-400 cm^{-1} on a Vertex 70 Bruker spectrophotometer on KBr pellets. ^1H NMR spectra were obtained on a JEOL JNM-LA 400 MHz spectrometer. ^1H NMR chemical shifts were referenced to the residual hydrogen signal of the deuterated solvents. Electronic absorptions were measured on a Lambda-20 Perkin-Elmer Spectrophotometer. Elemental analyses were performed on a Thermoquest EA1110 CHNS/O analyzer. GC was recorded on a Clarus 500 Perkin-Elmer gas chromatograph. The recrystallized compounds were powdered, washed several times with dry diethyl ether and dried in vacuum for at least 48 h prior to elemental analyses.

1.2 Materials. Solvents were dried by conventional methods, distilled under nitrogen and deoxygenated prior to use.¹ $\text{IrCl}_3 \cdot n\text{H}_2\text{O}$ (39% Ir) was purchased from Arora Matthey, India. The compounds $[\text{IrCl}(\text{COD})]_2$ ² and $[\text{Ir}(\text{COD})(\text{CH}_3\text{CN})_2][\text{BF}_4]$ ³ were synthesized following the literature procedures. The ligands 2-methyl-1.8-naphthyridine (NP-Me), 2-phenyl-1.8-naphthyridine (NP-Ph), and 2-ferrocenyl-1.8-naphthyridine (NP-Fc) were prepared by the Friedlander condensation of 2-aminonicotinaldehyde with corresponding acyl derivatives.⁴

(Caution: The reactions of carbon monoxides were carried out in a well vented fume hood.)

1.3 Syntheses

$[\text{Ir}(\text{COD})(\eta^1\text{-NP-Ph})_2][\text{BF}_4]$ (1). TIBF_4 (85 mg, 0.29 mmol) was added to an acetonitrile solution (10 mL) of $[\text{IrCl}(\text{COD})]_2$ (91 mg, 0.135 mmol) and the yellow mixture was stirred for 30 mins. The TlCl precipitate was removed by Schlenk filtration; NP-Ph (123 mg, 0.59 mmol) was added to the filtrate and stirred for 8 h at RT. The resulting solution was concentrated under vacuum and 15 mL of diethyl ether was added with stirring to induce precipitation. The solid residue obtained was washed with diethyl ether and dried in vacuum. Yield: 178 mg (82%, based on iridium). ^1H NMR (CDCl_3 , δ , ppm): 9.12 (s, 2H, NP), 8.68 (d, 4H, NP), 8.45(d, 2H, NP), 8.30 (d, 2H, NP), 8.14 (d, 2H, NP), 7.73 (m, 8H, Ph), 7.15 (m, 2H, Ph), 4.03 (br, 2H, COD), 3.76 (br, 2H, Me), 2.63 (s, 4H, COD), 1.85 (br, 2H, COD), 1.74 (br, 2H, COD), 1.56 (br, 4H, COD). IR (KBr) data (cm^{-1}): $\nu(\text{C-H, COD})$: 2931; $\nu(\text{BF}_4^-)$: 1057. Anal. Calcd for $\text{C}_{36}\text{H}_{32}\text{N}_4\text{B}_1\text{F}_4\text{Ir}_1$: C, 54.07; H, 4.03; N, 7.01. Found: C, 54.19; H, 4.10; N, 7.09. UV-Vis spectra [λ_{max} , nm (ϵ , $\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$)] (in CH_3CN): 246 (8.53×10^3), 325 (5.51×10^3), 411 (4.73×10^2), 466 (2.55×10^2).

$[\text{Ir}(\text{COD})(\eta^1\text{-NP-Fc})_2][\text{BF}_4]$ (2): TIBF_4 (83 mg, 0.28 mmol) was added to an acetonitrile solution (10 mL) of $[\text{IrCl}(\text{COD})]_2$ (90 mg, 0.134 mmol) and the yellow mixture was stirred for 30 mins. The TlCl precipitate was removed by Schlenk filtration, NP-Fc (170 mg, 0.54 mmol) was added to the

filtrate and stirred for 8 h at RT. The resulting orange solution was concentrated under vacuum and 15 mL of diethyl ether was added with stirring to induce precipitation. The solid residue obtained was washed with diethyl ether and dried in vacuum. Yield: 225 mg (90%, based on iridium). Crystals suitable for X-ray study was obtained by layering hexane on dichloromethane solution of the compound. ^1H NMR (CDCl_3 , δ , ppm): 9.11–8.83 (m, br, 6H, NP), 8.10–7.95 (m, 4H, NP), 4.21 (br, 18H, Fc), 4.08 (br, 2H, COD), 3.76 (br, 2H, Me), 2.69 (s, 2H, COD), 2.58 (s, 2H, COD), 1.91 (br, 2H, COD), 1.68 (br, 2H, COD), 1.50 (br, 4H, COD). IR (KBr pellet): ν (C–H, COD): 2931; ν (BF_4^-) 1058 cm^{-1} . Anal. Calcd for $\text{C}_{44}\text{H}_{40}\text{N}_4\text{B}_1\text{F}_4\text{Fe}_2\text{Ir}_1$: C, 52.04; H, 3.97; N, 5.52. Found: C, 51.92; H, 4.04; N, 5.58. UV-Vis spectra [λ_{max} , nm (ϵ , $\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$)] (in CH_3CN): 234 (7.78×10^3), 315 (6.61×10^3), 390 (5.55×10^2), 486 (br, 3.85×10^2).

$[\text{Ir}_2(\text{CO})_4(\mu\text{-NP-Ph})_2][\text{BF}_4]_2$ (3**).**

Carbonmonoxide was bubbled for 5 mins through a solution of **1** (25 mg, 0.037 mmol) in dichloromethane (10 mL). The initial orange solution turns green, and the dark green colored residue of $[\text{Ir}_2(\text{CO})_4(\mu\text{-NP-Ph})_2][\text{BF}_4]_2$ (**3**) precipitated out slowly from the reaction medium. The solution was filtered off through a filter paper-stripped cannula and the solid residue was washed with petroleum ether (3×5 mL) and dried in vacuum. Yield: 16 mg (90%, per iridium). ^1H NMR (CD_3CN , δ , ppm): 9.14 (s, 2H, NP), 8.81 (m, 2H, NP), 8.53 (m, 2H, NP), 8.36 (m, 4H, NP), 8.06 (m, 2H, Ph), 7.67 (d, 8H, Ph). IR (KBr) data (cm^{-1}): $\nu(\text{CO})$: 2063, 2002; $\nu(\text{BF}_4^-)$: 1072. Anal. Calcd for $\text{C}_{32}\text{H}_{20}\text{N}_4\text{O}_4\text{B}_2\text{F}_8\text{Ir}_2$: C, 35.50; H, 1.86; N, 5.18. Found: C, 35.61; H, 1.79; N, 5.29. ESI-MS: m/z 909 for $[\text{M}]^+$. UV-Vis spectra [λ_{max} , nm (ϵ , $\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$)] (in CH_3CN): 247, 328 (As compound **3** is not fully soluble in acetonitrile, “ ϵ ” values were not measured).

$[\text{Ir}(\text{CO})_2(\eta^1\text{-NP-Fc})_2][\text{BF}_4]$. Carbonmonoxide was bubbled for 5 mins through a 1,2-dichlorobenzene (10mL) solution of **2** (32 mg, 0.032 mmol) and the resultant red solution was stirred for 2 hrs at RT. It was then concentrated under vacuum and hexane (15 mL) was added with stirring to induce precipitation. The solid residue obtained was washed with diethyl ether and dried under vacuum. Crystals were grown by layering hexane onto the dichlorobenzene solution of the compound. Yield: 26 mg (86%, per iridium). ^1H NMR (CD_3CN , δ , ppm): 8.97 (br, 2H), 8.27 (br, m, 4H), 7.76 (br, m, 2H), 7.52 (br, m, 2H), 5.16 (br, s, 4H), 4.58 (s, 4H), 4.08 (br, m, 10H). IR (KBr) data (cm^{-1}): $\nu(\text{CO})$: 2074, 1999. Anal. Calcd for $\text{C}_{38}\text{H}_{28}\text{N}_4\text{O}_2\text{Fe}_2\text{Ir BF}_4$: C, 47.38; H, 2.93; N, 5.82. Found: C, 47.10; H, 2.63; N, 5.94. UV-Vis spectra [λ_{max} , nm (ϵ , $\text{dm}^3 \text{mol}^{-1} \text{cm}^{-1}$)] (in CH_3CN): 327 (4.24×10^3), 530 (2.61×10^2).

$[\text{Ir}(\text{COD})(\eta^1\text{-NP-Me})_2][\text{BF}_4]$. TlBF_4 (102 mg, 0.35 mmol) was added to an acetonitrile solution (10 mL) of $[\text{IrCl}(\text{COD})]_2$ (110 mg, 0.164 mmol). Immediate precipitation of TlCl took place and the

yellow mixture was stirred for 30 mins. The precipitate was removed by Schlenk filtration and NP-Me (100 mg, 0.69 mmol) was added to the filtrate. After stirring for 8 h at RT, the solution was concentrated under vacuum and 15 mL of diethyl ether was added with stirring to induce precipitation. The solid residue obtained was washed with diethyl ether and dried in vacuum. Analytically pure compound was obtained by recrystallization from a dichloromethane/hexane mixture. Yield: 180 mg (82%, based on iridium). ¹H NMR (CDCl₃, δ, ppm): 9.48 (s, 2H, NP), 8.28–8.21 (br, m, 4H, NP), 7.57–7.48 (br, m, 4H, NP), 4.1 (br, 2H, COD), 3.72 (br, 6H, Me), 3.02 (s, 6H, COD), 2.33 (br, 8H, COD), 1.67 (br, 2H, COD). IR (KBr) data (cm⁻¹): ν(C–H, COD): 2928; ν(BF₄⁻): 1058. Anal. Calcd for C₂₆H₂₈N₄B₁F₄Ir₁: C, 46.23; H, 4.18; N, 8.29. Found: C, 46.31; H, 4.11; N, 8.36. UV-Vis spectra [λ_{\max} , nm (ϵ , dm³ mol⁻¹ cm⁻¹)] (in CH₃CN): 255 (sh), 305 (3.25 × 10³), 366 (4.55 × 10²), 417 (3.84 × 10²).

1.4 GC Experiment

Carbonmonoxide was bubbled for 5 mins through a solution of **2** (30 mg, 0.031 mmol) and stirred for additional 6 h in dichloromethane (10 mL). Resulting purple solution was loaded on a silica gel (100–200 mesh) column and was eluted with diethyl ether. The liquid collected was injected into GC. 1,2-dichloroethane was identified by exact match with the retention time of the authentic sample.

2. X-ray Data Collections and Refinement. Single crystal X-ray structural studies were performed on a CCD Bruker SMART APEX diffractometer equipped with an Oxford Instruments low-temperature attachment. Data were collected at 100(2) K using graphite-monochromated Mo-K α radiation ($\lambda_{\alpha} = 0.71073 \text{ \AA}$). The frames were indexed, integrated and scaled using SMART and SAINT software package,⁵ and the data were corrected for absorption using the SADABS program.⁶ The structures were solved and refined using SHELX suite of programs⁷ while additional crystallographic calculations were performed by the programs PLATON.⁸ Figures were drawn using ORTEP32.⁹ The hydrogen atoms were included into geometrically calculated positions in the final stages of the refinement and were refined according to ‘riding model’. For compound **4**, an empirical absorption correction was applied using XABS2.¹⁰ All non-hydrogen atoms were refined with anisotropic thermal parameters. The ‘SQUEEZE’ option in PLATON was used to remove a disordered solvent molecule from the overall intensity data of compound **4**. For compound **5**, all non-hydrogen atoms of the diiridium complex except N1, C15, C17, C18 and C27 were refined with anisotropic thermal parameters. Anisotropic treatment of these five atoms resulted non-positive definite displacement tensors and were therefore subjected to isotropic refinement. The CH₂Cl₂ molecule was found to be disordered and was modeled satisfactorily. The disordered Cl atoms were refined isotropically. Hydrogens of the solvates were not included in the structure. The ‘SQUEEZE’

option in PLATON was used to remove a disordered solvent molecule from the overall intensity data of compound **5**. Pertinent crystallographic data for compounds **4** and **5** are summarized in Table S1.

3. Theoretical Studies. Calculations were performed using density functional theory (DFT) with Becke's three parameter hybrid exchange functional¹¹ and the Lee-Yang-Parr correlation functional (B3LYP).¹² Atomic coordinates of the [Ir₂Cl₄(CO)₄] unit were taken from the single-crystal X-ray structure and were optimized in C₂ symmetry. The atomic coordinates of two axially bound NP-Fc were omitted from the single-crystal X-ray structure for optimization. Vibrational frequency analysis was performed on the optimized geometry which verified that the optimized structure was a local minimum on the potential energy surface. The double- ζ basis set of Hay and Wadt (LanL2DZ) with a small core (1s2s2p3s3p3d4s4p4d) effective core potential (ECP)¹³ was used for the Ir. The ligand atoms H, C and O atoms were described using the 6-31G(d,p) basis sets, and 6-311++G (3df, 3pd) basis sets for Cl atom was employed. All calculations were performed with the Gaussian 03 (G03) suite of programs.¹⁴ Gaussview 3.0 was used for generating the orbital plots.¹⁵

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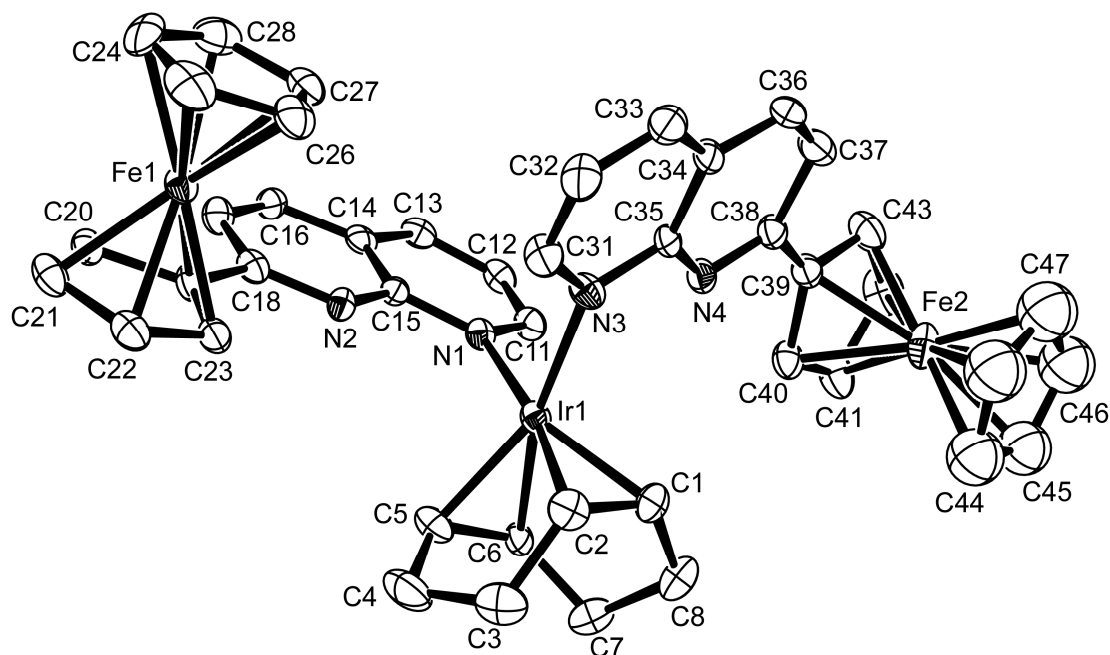


Figure S2. ORTEP diagram (50% probability thermal ellipsoids) of the cationic unit $[\text{Ir}(\text{COD})(\eta^1\text{-NP-Fc})_2]^+$ in compound **2** with important atoms labeled. Hydrogen atoms omitted for the sake of clarity. Crystal data for **2**: $\text{C}_{44}\text{H}_{40}\text{BF}_4\text{Fe}_2\text{IrN}_4$, $M = 1015.51$, monoclinic, space group $P2_1/c$ (No. 14), $a = 18.941(6)$, $b = 20.273(6)$, $c = 11.878(4)$ Å, $\beta = 106.025(5)^\circ$, $V = 4384(2)$ Å³, $Z = 4$, $\rho_c = 1.539$ g/cm³, $F_{000} = 2008$, $2\theta_{\text{max}} = 52.7^\circ$, 24389 reflections collected, 8872 unique ($R_{\text{int}} = 0.0561$). Final $\text{Goof} = 0.942$, $R1 = 0.0561$, $wR2 = 0.1402$, R indices based on 6091 reflections with $I > 2\sigma(I)$ (refinement on F^2), 440 parameters, 0 restraints, $\mu = 3.732$ mm⁻¹.

Important Bond distances (Å) and angles (deg): Ir1-C5 2.083(8), Ir1-C1 2.100(8), Ir1-N1 2.101(6), Ir1-C2 2.113(9), Ir1-N3 2.121(6), Ir1-C6 2.128(7), N1-Ir1-N3 92.4(2).

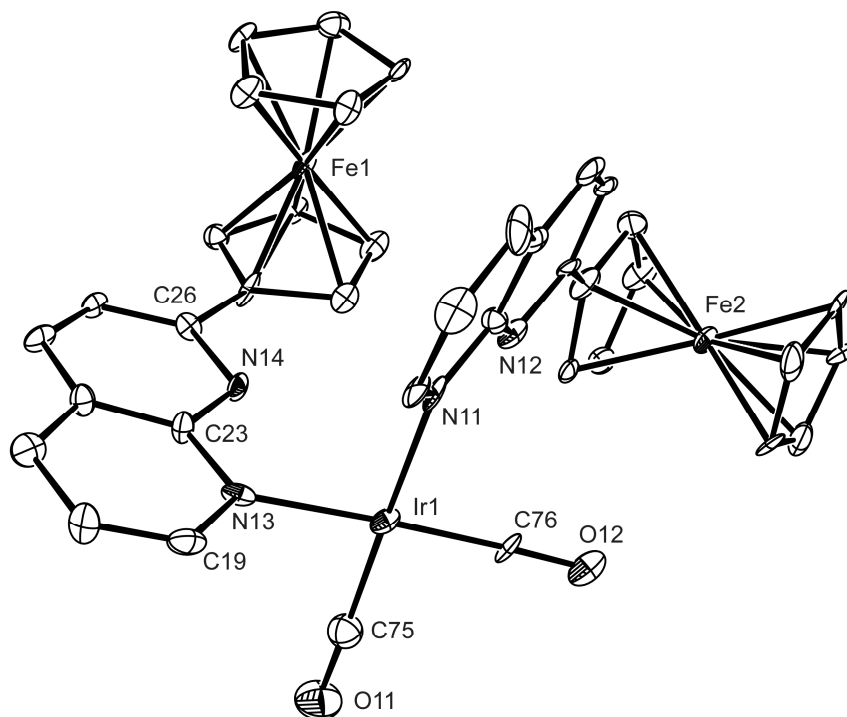


Figure S3. ORTEP diagram (40% probability thermal ellipsoids) of the cationic unit of $[\text{Ir}(\text{CO})_2(\mu\text{-NP-Fc})_2][\text{BF}_4]$ with important atoms labeled. Hydrogen atoms omitted for the sake of clarity. Crystal data for $[\text{Ir}(\text{CO})_2(\mu\text{-NP-Fc})_2][\text{BF}_4] \cdot 0.5\text{C}_6\text{H}_4\text{Cl}_2$: $\text{C}_{41}\text{H}_{30}\text{BClF}_4\text{Fe}_2\text{IrN}_4\text{O}_2$, $M = 1036.85$, triclinic, space group $P-1$ (No. 2), $a = 12.165(2)$, $b = 18.979(4)$, $c = 20.639(4)$ Å, $\alpha = 75.029(3)$, $\beta = 89.290(4)$, $\gamma = 80.419(4)^\circ$, $V = 4536.8(16)$ Å³, $Z = 4$, $\rho_c = 1.518$ g/cm³, $F_{000} = 2028$, $2\theta_{\text{max}} = 52.7^\circ$, 25929 reflections collected, 18044 unique ($R_{\text{int}} = 0.0804$). Final $\text{Goof} = 0.874$, $RI = 0.0868$, $wR2 = 0.1953$, R indices based on 8355 reflections with $I > 2\sigma(I)$ (refinement on F^2), 974 parameters, 0 restraints, $\mu = 3.668$ mm⁻¹.

Important Bond distances (Å) and angles (deg): Ir1-C75 1.778(19), Ir1-C76 1.788(13), Ir1-N13 2.076(12), Ir1-N11 2.130(12), N13-Ir1-N11 88.8(4), C75-Ir1-C76 89.6(7), C75-Ir1-N13 89.7(6), C76-Ir1-N13 176.9(5), C75-Ir1-N11 172.8(7), C76-Ir1-N11 91.5(6).

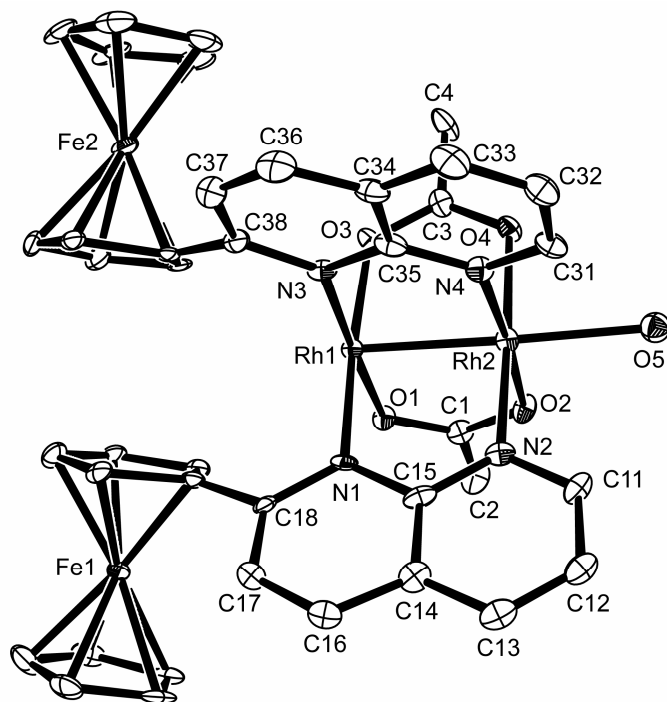


Figure S4. ORTEP diagram (50% probability thermal ellipsoids) of the cationic unit $cis\text{-}[\text{Rh}_2(\mu\text{-NP-Fc})_2(\text{OAc})_2(\text{H}_2\text{O})]^{2+}$ in compound $cis\text{-}[\text{Rh}_2(\mu\text{-NP-Fc})_2(\text{OAc})_2(\text{H}_2\text{O})][\text{SO}_3\text{CF}_3]_2$ with important atoms labeled. Hydrogen atoms omitted for the sake of clarity.

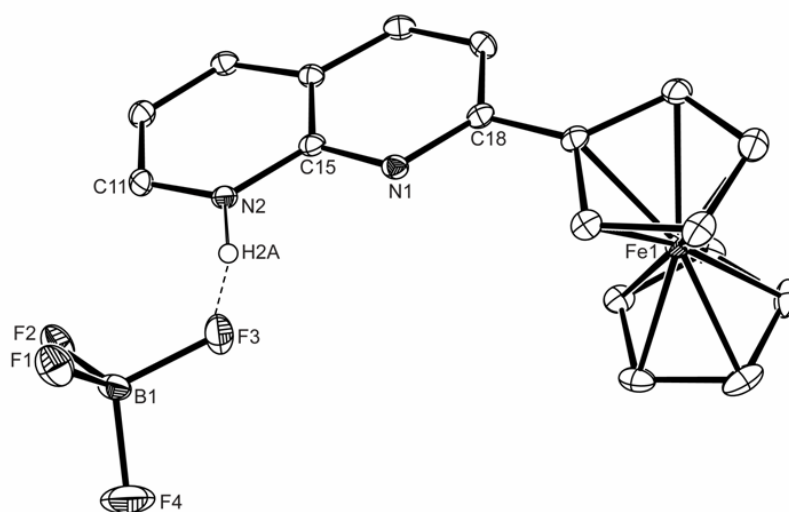


Figure S5. ORTEP diagram (40% probability thermal ellipsoids) of the molecular structure of [H.NP-Fc][BF₄] with important atoms labeled. Hydrogen atoms omitted for the sake of clarity. Crystal data for [H.NP-Fc][BF₄].CH₂Cl₂: C₁₉H₁₇BCl₂F₄FeN₂, $M = 486.91$, triclinic, space group $P-1$ (No. 2), $a = 10.1056(8)$, $b = 10.2579(9)$, $c = 11.3678(10)$ Å, $\alpha = 103.9290(10)$, $\beta = 102.5580(10)$, $\gamma = 112.9230(10)^\circ$, $V = 987.55(15)$ Å³, $Z = 2$, $\rho_c = 1.637$ g/cm³, $F_{000} = 492$, $2\theta_{\max} = 56.6^\circ$, 6593 reflections collected, 4662 unique ($R_{\text{int}} = 0.0164$). Final $GooF = 0.992$, $RI = 0.0478$, $wR2 = 0.0903$, R indices based on 4011 reflections with $I > 2\sigma(I)$ (refinement on F^2), 266 parameters, 0 restraints, $\mu = 1.079$ mm⁻¹.

Important Bond distances (Å) and angles (deg): N2-H2A 0.816, N2-F3 2.860(3), F3-H2A 2.051, N2-H2A-F3 171.09.

Table S1. Crystallographic Data and Refinement Parameters for compounds **4** and **5•2CH₂Cl₂**.

	4	5•2CH₂Cl₂
Empirical formula	C ₂₂ H ₁₆ B ₂ F ₈ Ir ₂ N ₄ O ₄	C ₄₂ H ₂₈ Cl ₈ Fe ₂ Ir ₂ N ₄ O ₄
Formula weight	958.41	1432.38
Crystal system	Orthorhombic	Monoclinic
Space group	Pbcn	C2/c
a, Å	10.8097(7)	16.473(2)
b, Å	32.184(2)	14.541(2)
c, Å	19.7274(14)	20.961(3)
α, deg		
β, deg		97.097(2)
γ, deg		
V, Å ³	6863.2(8)	4982.5(12)
Z	8	4
Collection temperature(K)	100(2)	100(2)
ρ _{calcd} , g cm ⁻³	1.855	1.910
μ, mm ⁻¹	7.821	6.367
F(000)	3552	2728
R _{int}	0.000	0.0729
Reflections		
Collected	5861	13966
Independent	5861	5057
observed [I > 2σ(I)]	4497	3660
No. of variables	383	254
Goodness-of-fit	0.973	0.991
Final R indices [I > 2σ(I)] ^a	R ₁ =0.0394 wR ₂ =0.0843	R ₁ =0.0554 wR ₂ =0.1187
R indices (all data) ^a	R ₁ =0.0585 wR ₂ =0.0900	R ₁ =0.0820 wR ₂ =0.1277

$$^a R_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|} \text{ with } F_o^2 > 2\sigma(F_o^2). \quad wR_2 = \left[\frac{\sum w(|F_o|^2 - |F_c|^2)^2}{\sum |F_o|^2} \right]^{1/2}.$$

Table S2. Relevant Metrical Parameters of Compound **4**.

Bond Lengths (Å)			
Ir1–Ir1	2.8151(7)	Ir2–Ir2	2.8051(7)
Ir1–N11	2.123(6)	Ir2–N21	2.133(7)
Ir1–N12	2.116(7)	Ir2–N22	2.119(7)
Ir1–C1	1.850(10)	Ir2–C3	1.838(10)
Ir1–C2	1.849(10)	Ir2–C4	1.864(11)
Bond Angles (deg)			
N11–Ir1–Ir1	86.63(17)	N21–Ir2–Ir2	79.61(19)
N12–Ir1–Ir1	80.51(18)	N22–Ir2–Ir2	85.35(17)
C1–Ir1–Ir1	98.2(3)	C3–Ir2–Ir2	95.0(3)
C2–Ir1–Ir1	104.3(3)	C4–Ir2–Ir2	105.8(3)
N12–Ir1–C2	173.4(3)	N22–Ir2–C3	178.8(3)
N11–Ir1–C2	89.6(3)	N21–Ir2–C4	174.2(3)
N12–Ir1–C1	93.3(3)	N22–Ir2–C4	91.1(3)
N11–Ir1–N12	86.1(2)	N21–Ir2–N22	87.3(2)
N11–Ir1–C1	175.0(3)	N21–Ir2–C3	91.6(3)
C1–Ir1–C2	90.5(4)	C3–Ir2–C4	90.0(4)

Table S3. Relevant Metrical Parameters of Compound **5**.

Bond Lengths (Å)			
Ir1–Ir1	2.7121(8)	Ir1–Cl2	2.386(3)
Ir1–N1	2.183(7)	Ir1–C1	1.871(11)
Ir1–Cl1	2.378(2)	Ir1–C2	1.892(10)
Bond Angles (deg)			
N1–Ir1–Ir1	178.8(2)	C2–Ir1–Cl1	177.6(3)
C1–Ir1–Ir1	88.2(3)	N1–Ir1–Cl2	87.5(2)
C2–Ir1–Ir1	87.9(3)	C1–Ir1–Cl2	178.6(3)
Cl1–Ir1–Ir1	92.62(6)	C2–Ir1–Cl2	87.6(3)
Cl2–Ir1–Ir1	91.50(6)	C1–Ir1–N1	92.8(3)
Cl1–Ir1–Cl2	90.09(9)	C2–Ir1–N1	92.7(3)
N1–Ir1–Cl1	86.7(2)	C1–Ir1–C2	93.8(4)
C1–Ir1–Cl1	88.6(3)		
Torsional Angles (deg)			
Cl1–Ir1–Ir1–Cl1	48.54(13)	C1–Ir1–Ir1–C1	128.4(6)
Cl2–Ir1–Ir1–Cl2	131.15(12)	C2–Ir1–Ir1–C2	44.1(6)
Cl1–Ir1–Ir1–Cl2	138.69(9)	C1–Ir1–Ir1–C2	137.8(4)

Table S4. Relevant Metrical Parameters of $[\text{Ir}_2\text{Cl}_4(\text{CO})_4]$ (optimized in C2 symmetry) obtained from DFT calculation.

Bond Lengths (Å)			
Ir1–Ir1	2.6834	Ir1–C1	1.9120
Ir1–Cl1	2.3293	Ir1–C2	1.9037
Ir1–Cl2	2.3516		
Bond Angles (deg)			
C1–Ir1–Ir1	89.7879	Cl2–Ir1–Ir1	95.1977
C2–Ir1–Ir1	91.7138	Cl1–Ir1–Cl2	89.1977
Cl1–Ir1–Ir1	99.9033	C1–Ir1–C2	95.2311
Torsional Angles (deg)			
Cl1–Ir1–Ir1–Cl1	53.2047	C1–Ir1–Ir1–C1	121.0411
Cl2–Ir1–Ir1–Cl2	126.6098	C2–Ir1–Ir1–C2	48.5045
Cl1–Ir1–Ir1–Cl2	143.297	C1–Ir1–Ir1–C2	143.731

Table S5. B3LYP optimized co-ordinates of $[\text{Ir}_2\text{Cl}_4(\text{CO})_4]$ in C_2 symmetry for DFT calculation.

	x	y	z
Ir	0.00000000	0.00000000	0.00000000
Cl	2.32930054	0.00000000	0.00000000
Cl	0.03292810	2.35138602	0.00000000
Ir	-0.46178032	-0.23665492	-2.63274234
O	0.16862382	-3.03199394	0.30111410
O	-2.95755859	0.22134238	0.68544173
C	-1.86306438	0.11202688	0.37473852
C	0.09331700	-1.90405523	0.14757073
Cl	0.82307423	-2.12323430	-3.09707848
Cl	-2.34808416	-1.62058372	-2.39462601
O	2.02692221	1.40822170	-3.27526200
O	-2.40909792	2.10233507	-2.68801984
C	-1.65489342	1.24663474	-2.61483206
C	1.10243504	0.80217281	-2.99326800