Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Heterobimetallic Complexes of IrM (M = Fe^{II}, Co^{II}, and Ni^{II}) Core and Bridging 2-(Diphenylphosphino)pyridine: Electronic Structure and Electrochemical Behavior

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Contents

NMR Spectra of 1 – 4

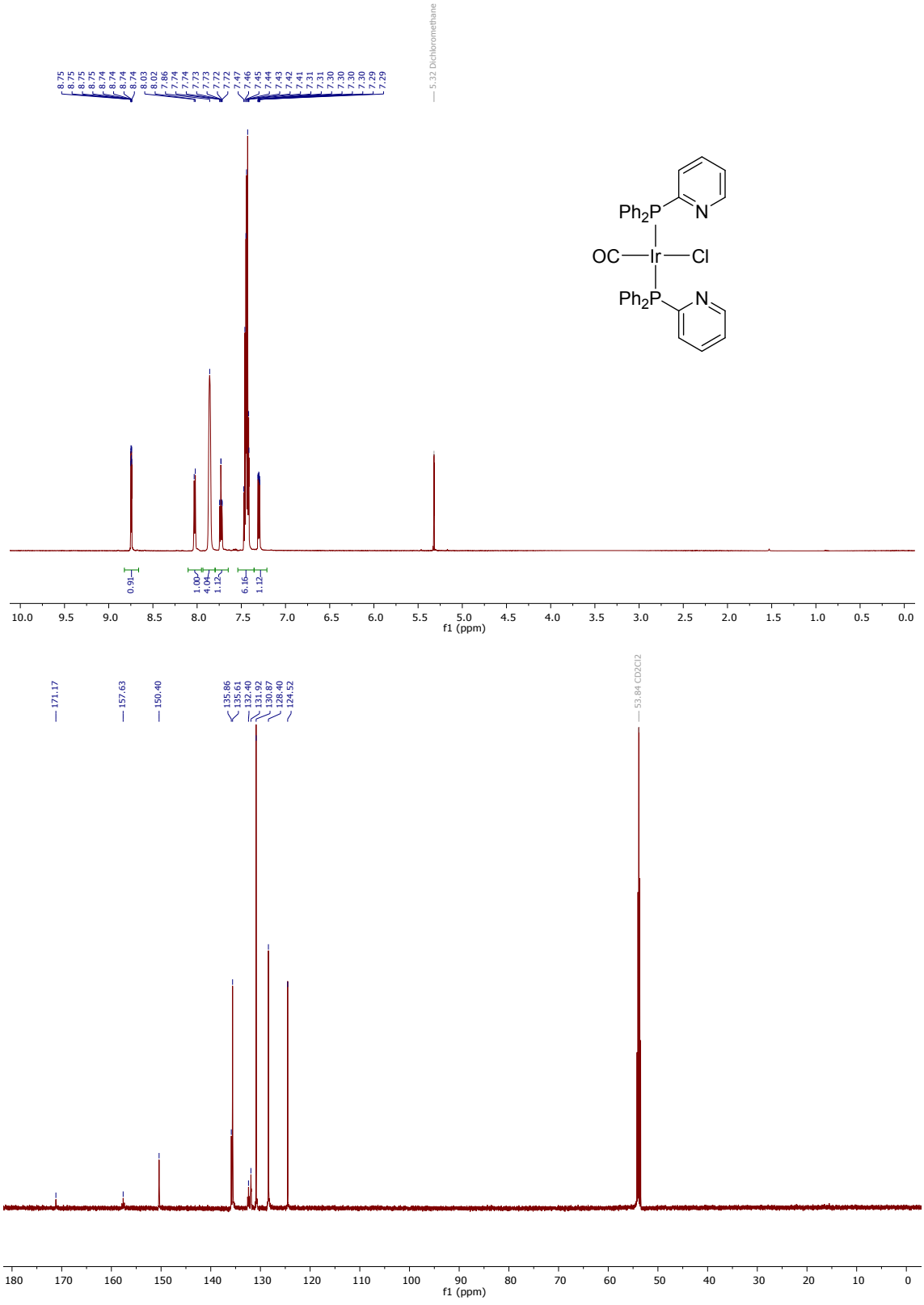


Figure S1. ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of **1** in CD_2Cl_2.

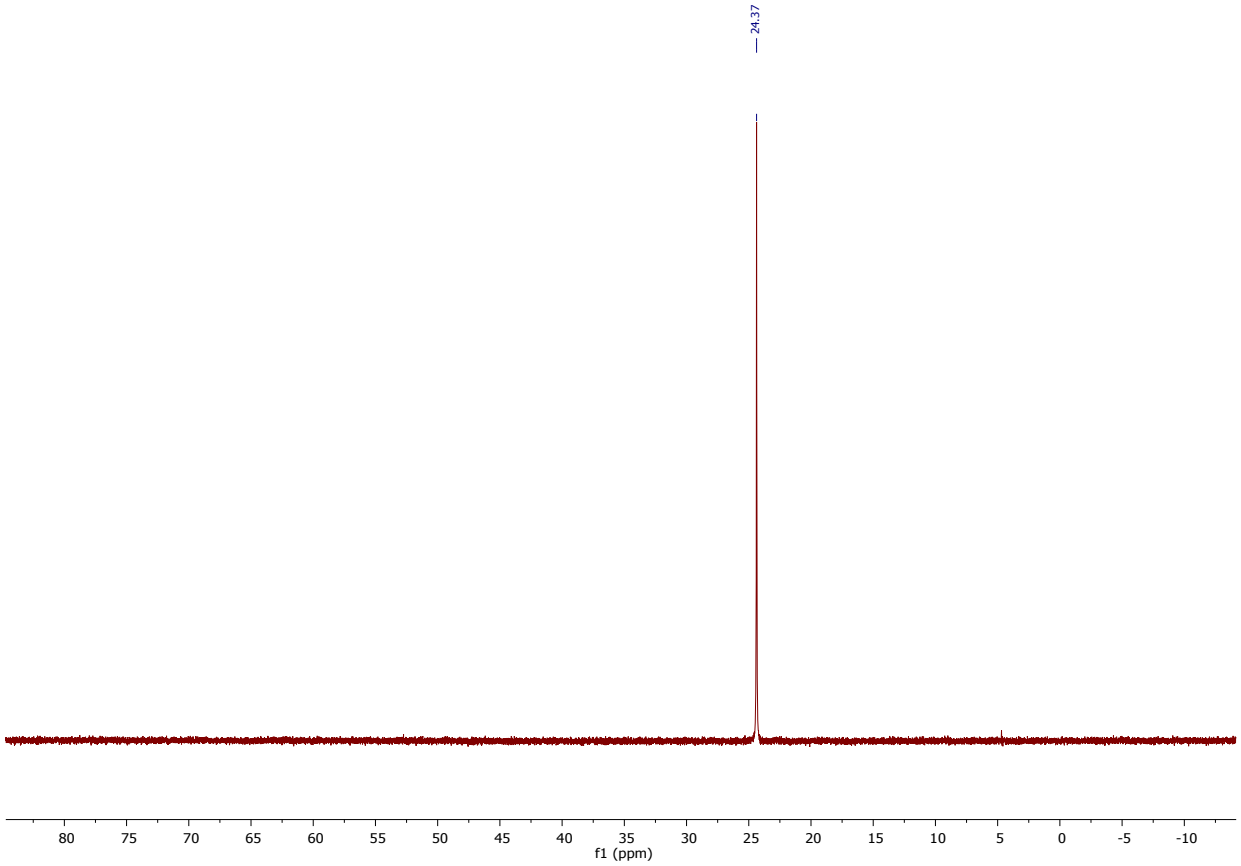


Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum of **1** in CD_2Cl_2.

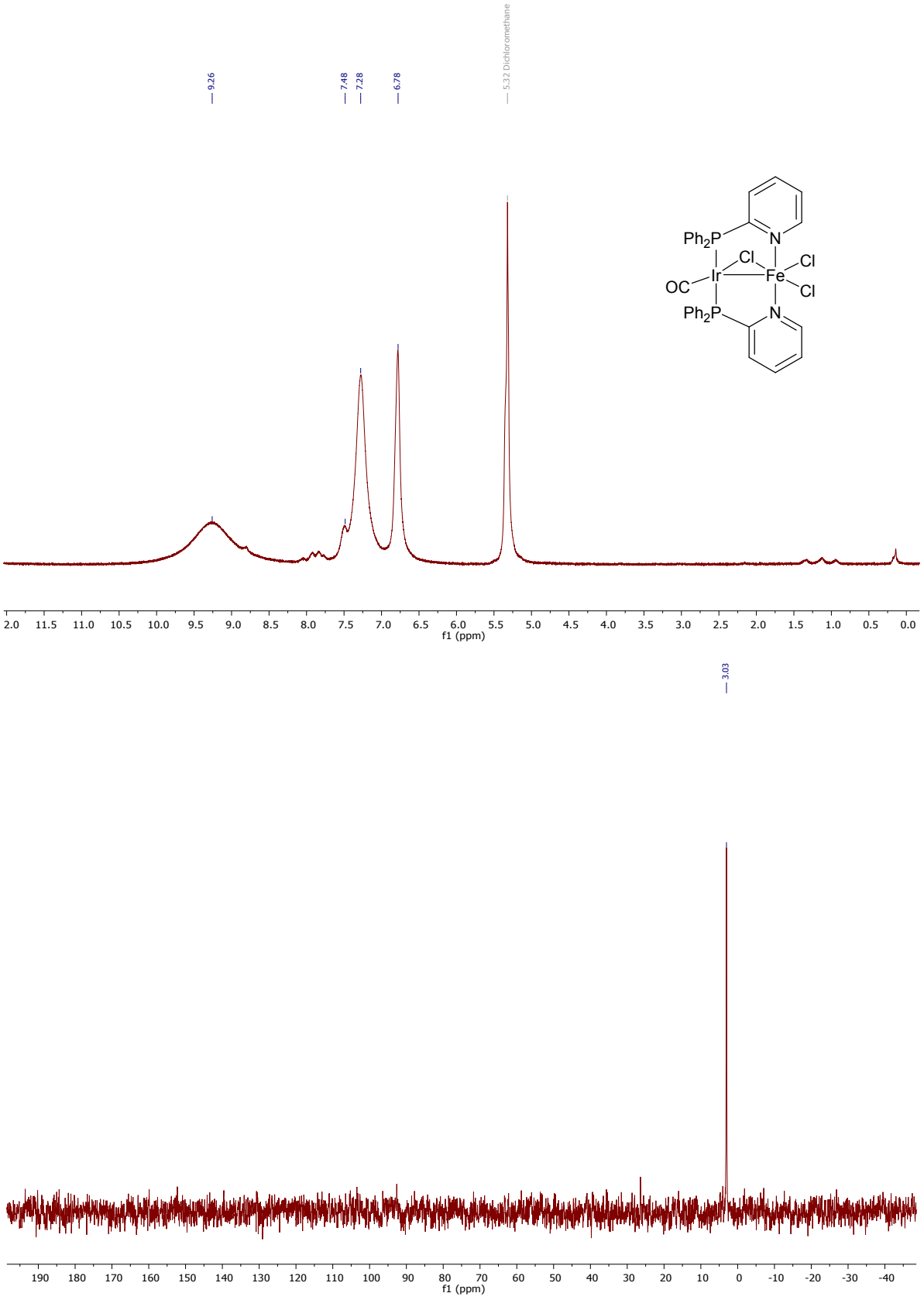


Figure S3. ^{1}H and $^{31}P\{^{1}H\}$ NMR spectra of **2** in CD_2Cl_2.

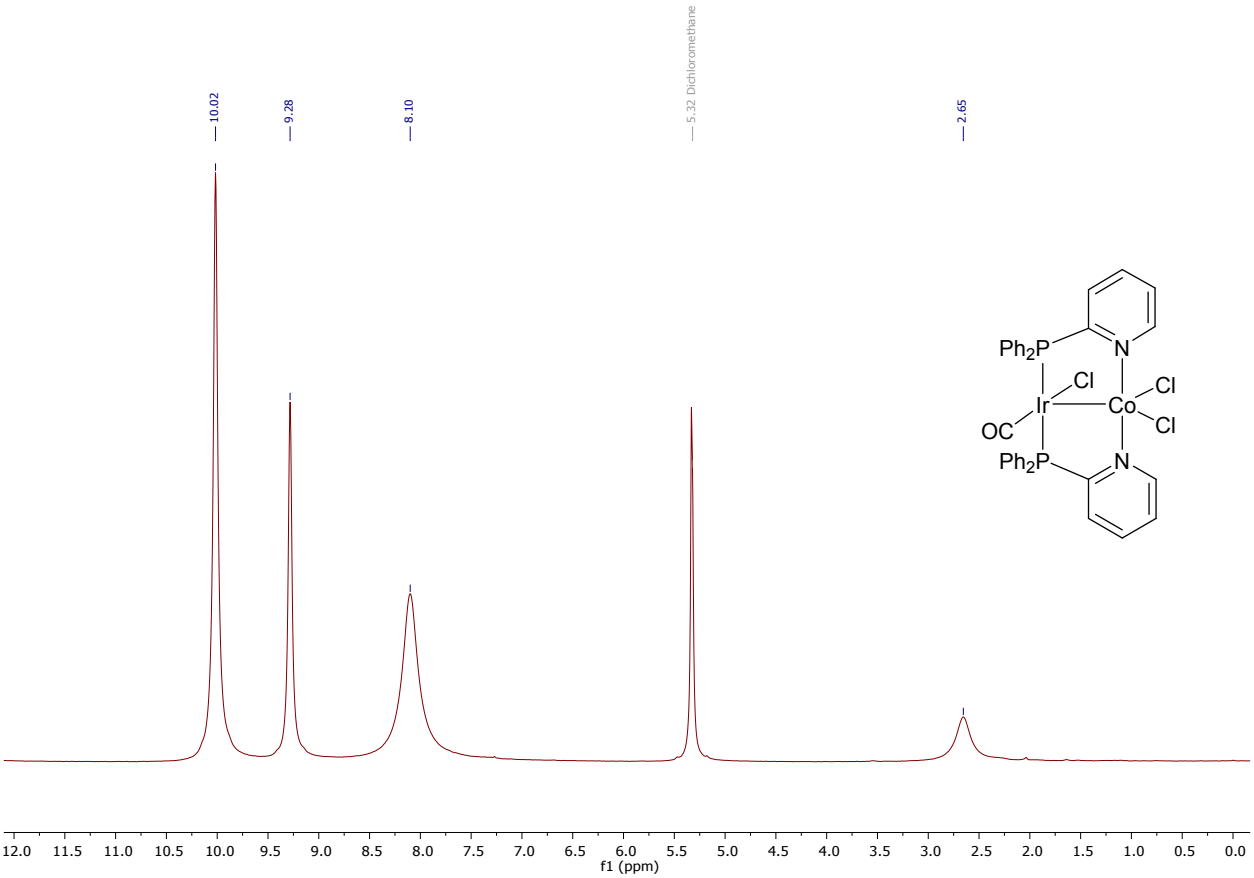


Figure S4. ^{1}H NMR spectrum of **3** in CD_2Cl_2.

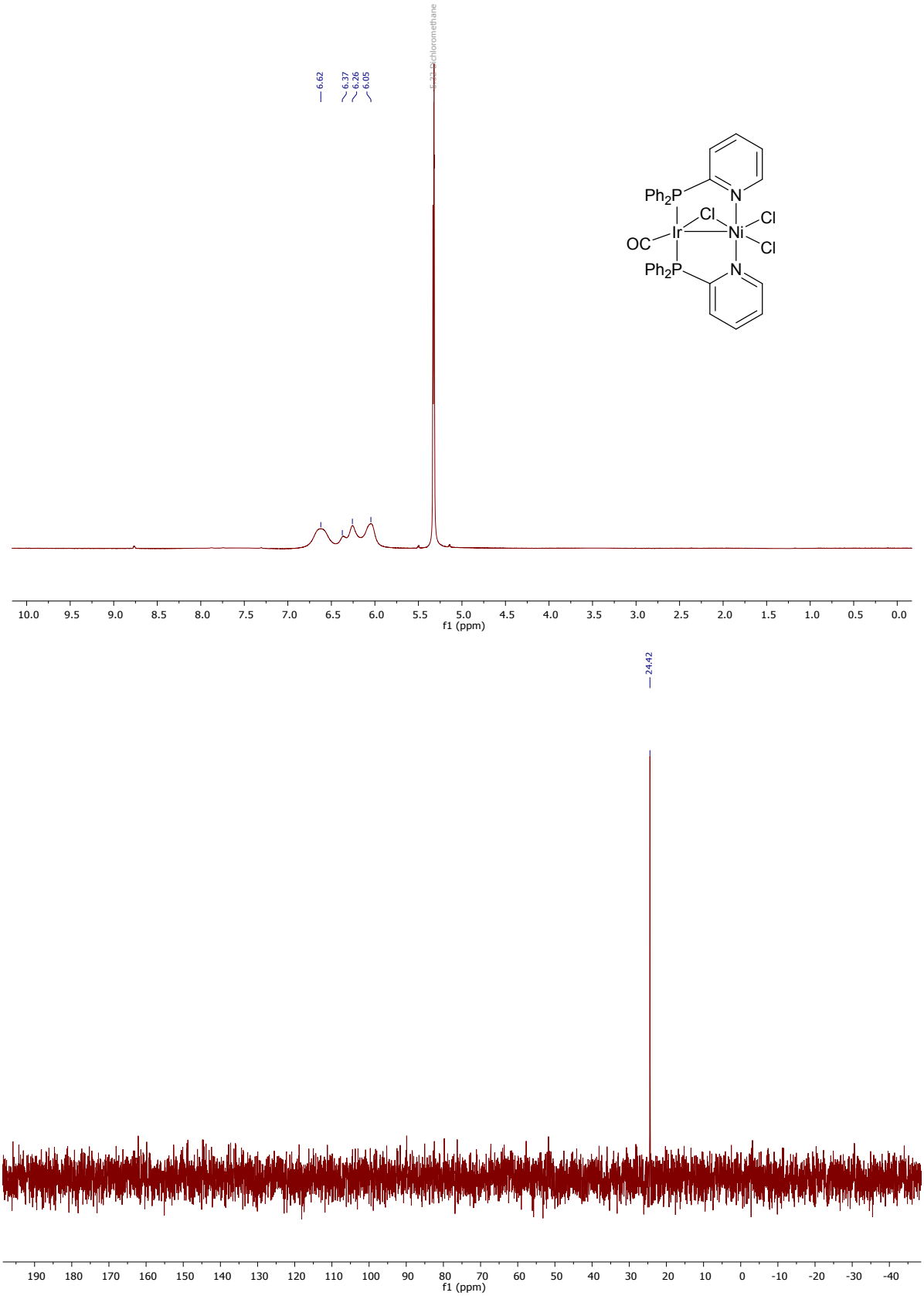
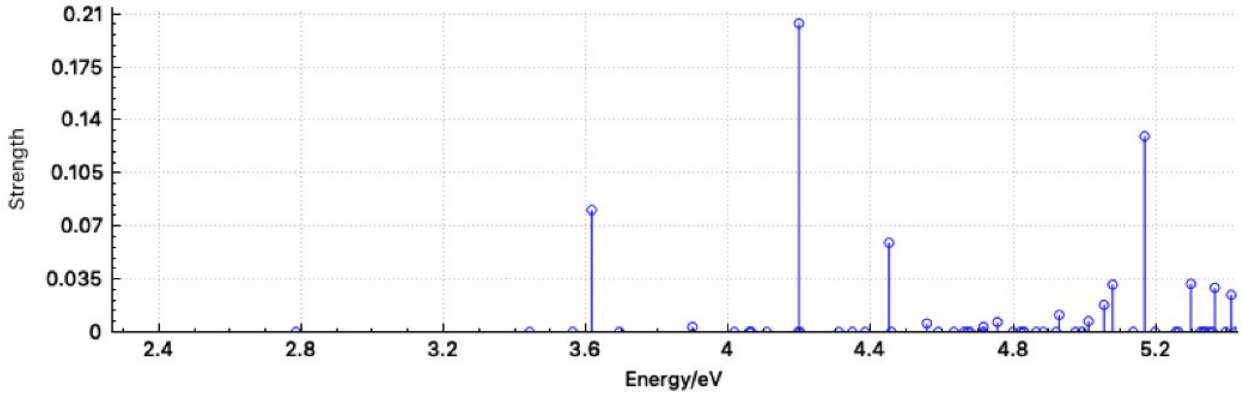


Figure S5. ^{1}H and $^{31}P\{^{1}H\}$ NMR spectra of **4** in CD_2Cl_2.

Computational Studies

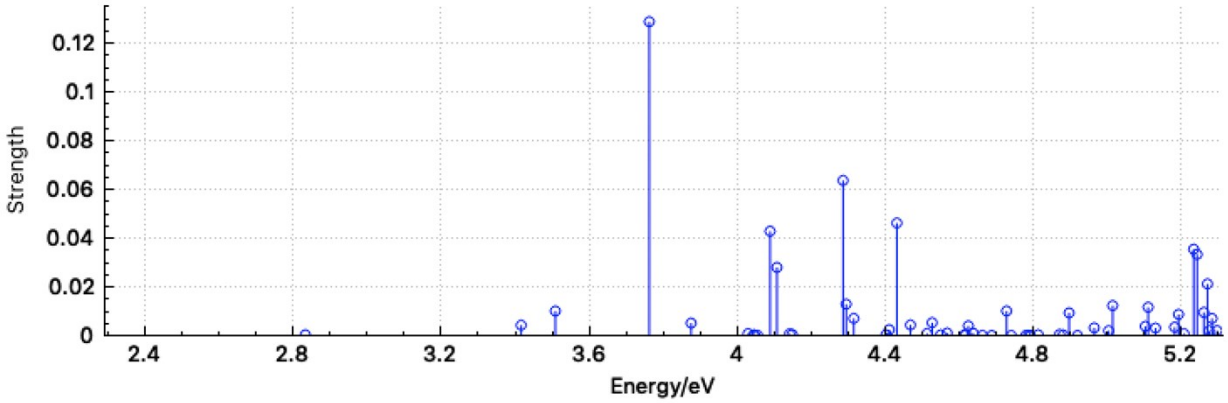
(TDDFT-based UV-vis spectra, corresponding excitation energies, and oscillator strengths for **1** – **4**)

Complex 1



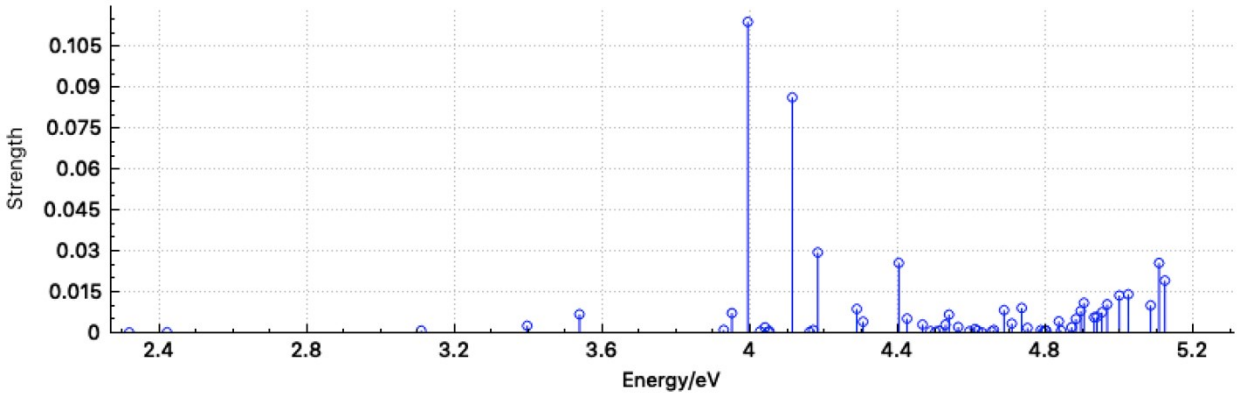
State	Excitation energy (eV)	<S**2>	Strength
1	2.79	2	0
2	3.44	2	0
3	3.56	2	0
4	**3.62**	**0**	**0.08**
5	3.69	2	0
6	3.90	0	0
7	4.02	2	0
8	4.06	2	0
9	4.06	2	0
10	4.06	2	0
11	4.11	2	0
12	4.20	2	0
13	**4.20**	**0**	**0.20**
14	4.20	2	0
15	4.31	2	0
16	4.35	2	0
17	4.38	2	0
18	4.45	0	0.06
19	4.46	2	0
20	4.56	0	0.01

Complex 2



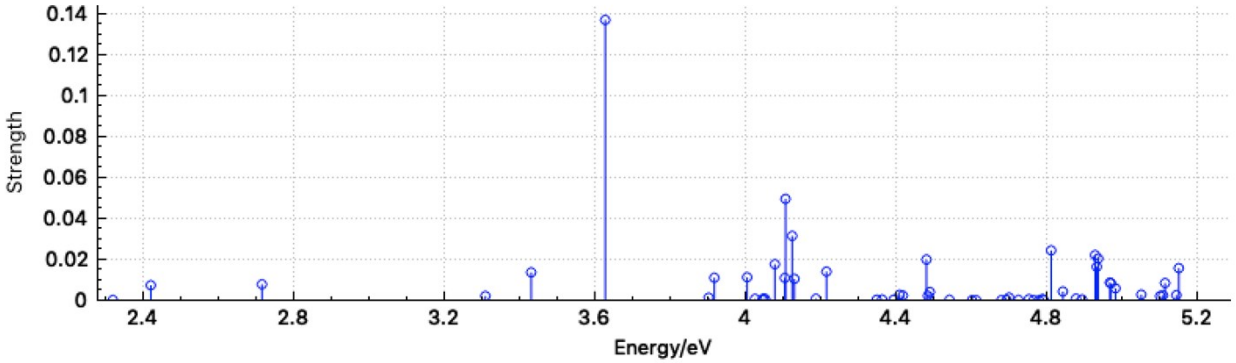
State	Excitation energy (eV)	<S**2>	Strength
1	0.40	6.02	0
2	0.52	6.02	0
3	0.71	6.02	0
4	1.50	6.02	0
5	2.83	7.62	0
6	3.42	7.64	0
7	3.51	7.52	0.01
8	**3.76**	**6.18**	**0.13**
9	3.88	7.57	0.01
10	4.03	7.99	0
11	4.05	7.95	0
12	4.05	8.01	0
13	4.06	8.00	0
14	4.09	6.84	0.04
15	4.11	7.03	0.03
16	4.14	7.97	0
17	4.15	7.98	0
18	4.29	6.20	0.06
19	4.29	7.45	0.01
20	4.31	6.48	0.01

Complex 3



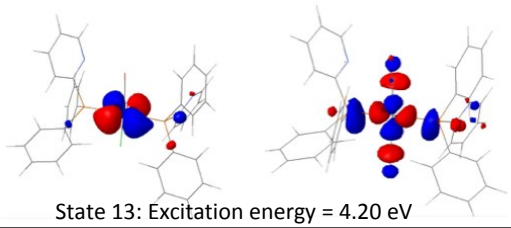
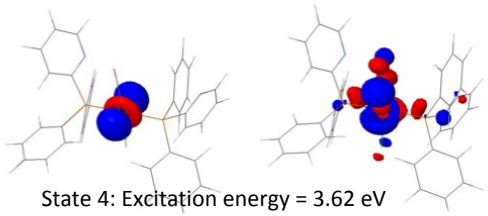
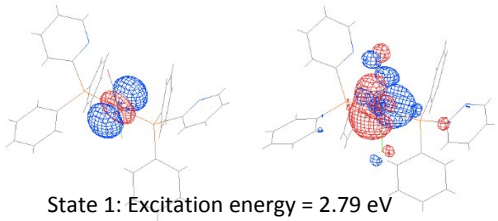
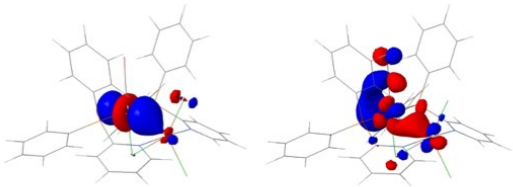
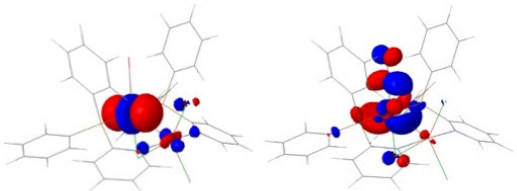
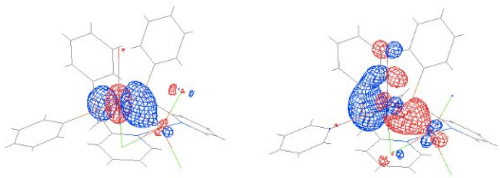
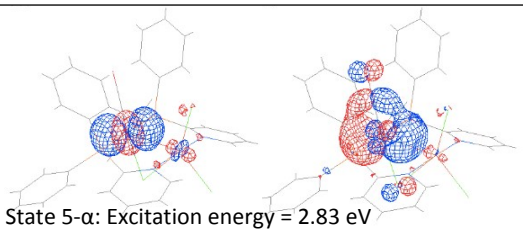
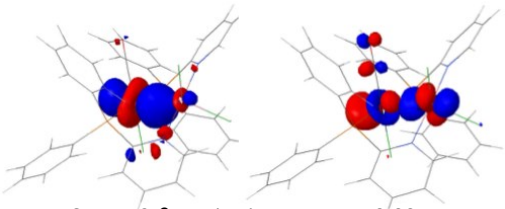
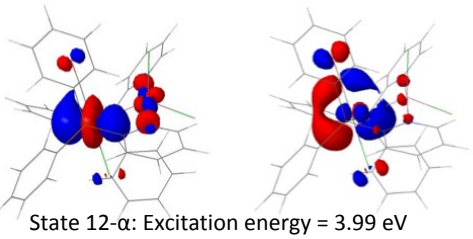
State	Excitation energy (eV)	<S**2>	Strength
1	0.15	3.77	0
2	0.15	3.77	0
3	0.83	3.77	0
4	0.90	3.77	0
5	2.32	3.77	0
6	2.42	3.77	0
7	3.11	5.10	0
8	3.40	5.38	0
9	3.54	5.24	0.01
10	3.93	3.90	0
11	3.95	4.90	0.01
12	**3.99**	**3.91**	**0.11**
13	4.03	5.75	0
14	4.04	5.71	0
15	4.05	5.75	0
16	4.05	5.75	0
17	4.11	4.20	0.09
18	4.16	5.75	0
19	4.17	5.71	0
20	4.18	3.98	0.03

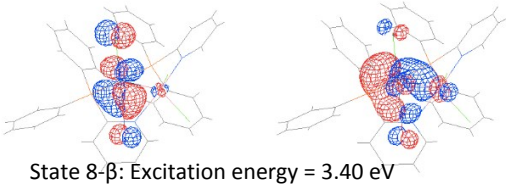
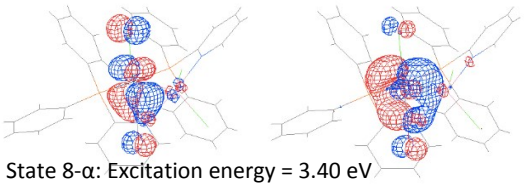
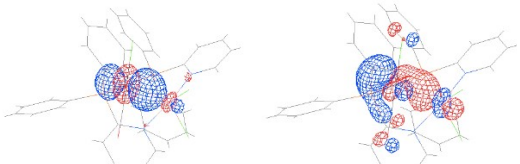
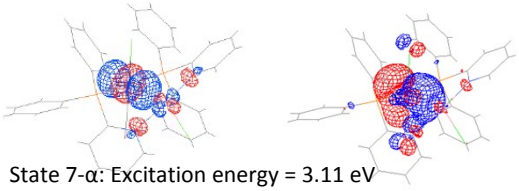
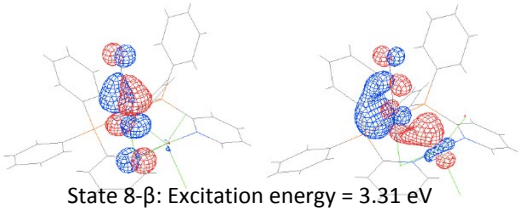
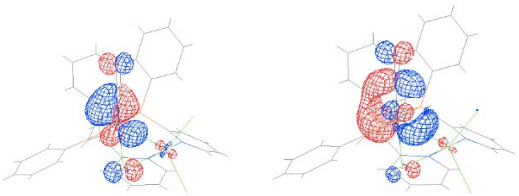
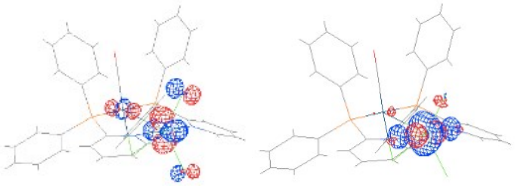
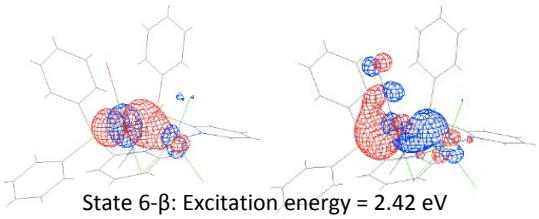
Complex 4



State	Excitation energy (eV)	<S**2>	Strength
1	1.02	2.02	0
2	1.46	2.01	0
3	1.51	2.01	0
4	2.21	2.01	0
5	2.32	2.01	0
6	2.42	2.06	0.01
7	2.72	3.33	0.01
8	3.31	3.34	0
9	3.43	3.24	0.01
10	**3.63**	**2.31**	**0.14**
11	3.90	2.70	0
12	3.92	3.57	0.01
13	4.01	2.49	0.01
14	4.03	3.99	0
15	4.05	3.99	0
16	4.05	3.97	0
17	4.05	3.95	0
18	4.08	2.26	0.02
19	4.11	3.57	0.01
20	4.11	2.86	0.05

Table S1. The dominant natural transition orbital pairs for **1** – **4**.

Compound	Hole → Particle(1)	Hole → Particle(2)
1	 State 13: Excitation energy = 4.20 eV	
	 State 4: Excitation energy = 3.62 eV	
	 State 1: Excitation energy = 2.79 eV	
2	 State 8-β: Excitation energy = 3.76 eV	 State 8-α: Excitation energy = 3.76 eV
	 State 5-β: Excitation energy = 2.83 eV	 State 5-α: Excitation energy = 2.83 eV
3	 State 12-β: Excitation energy = 3.99 eV	 State 12-α: Excitation energy = 3.99 eV

	 State 8-β: Excitation energy = 3.40 eV	 State 8-α: Excitation energy = 3.40 eV
	 State 7-β: Excitation energy = 3.11 eV	 State 7-α: Excitation energy = 3.11 eV
4	State 10-β: Excitation energy = 3.63 eV	State 10-α: Excitation energy = 3.63 eV
	 State 8-β: Excitation energy = 3.31 eV	 State 8-α: Excitation energy = 3.31 eV
	 State 6-β: Excitation energy = 2.42 eV	 State 6-β: Excitation energy = 2.42 eV

Electrochemical Studies

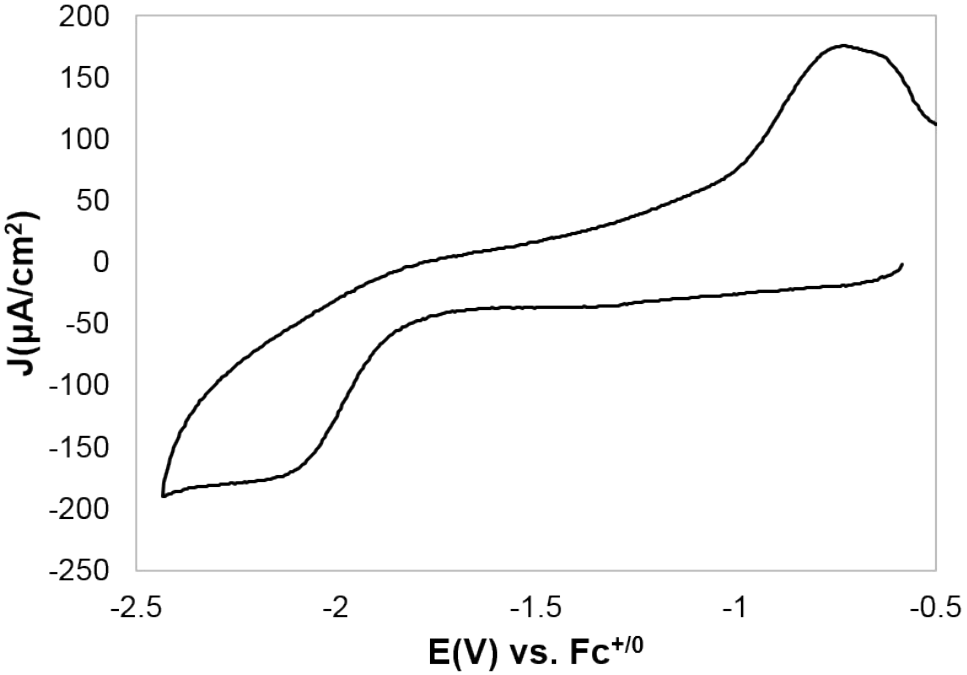


Figure S6. Cyclic voltammogram of **2** under N_2 in THF with 0.1 M [nBu$_4$N][PF$_6$] as the supporting electrolyte (scan rate: 100mV s^{-1}). One electrochemically irreversible cathodic couple is observed; however, the electrode is passivated with subsequent scans, and the feature disappears.

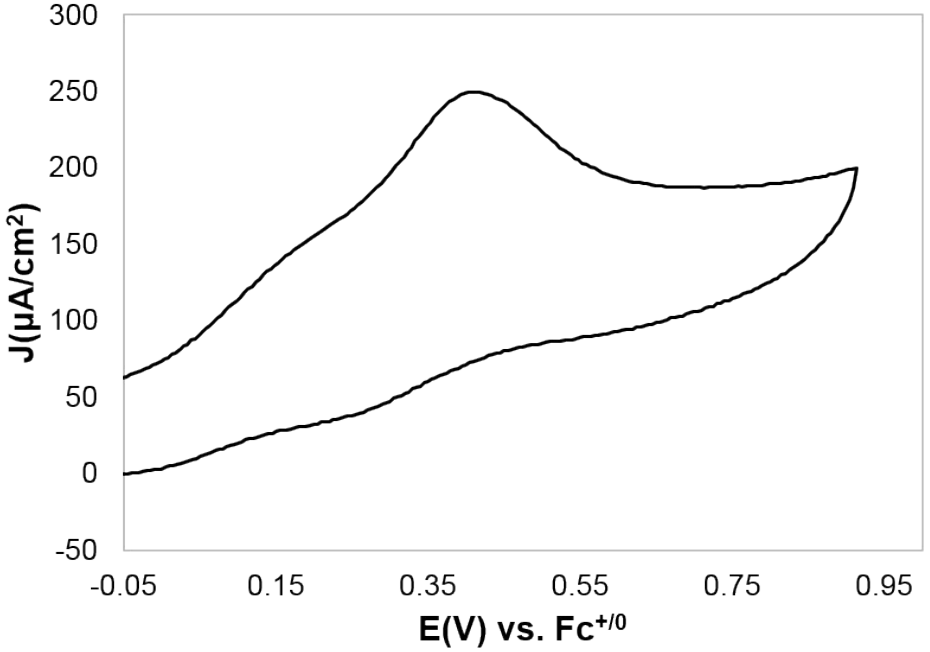


Figure S7. Cyclic voltammogram of **2** under N_2 in THF with 0.1 M [nBu$_4$N][PF$_6$] as the supporting electrolyte (scan rate: 100mV s^{-1}). One irreversible oxidative feature is observed, but the electrode becomes passivated with subsequent scans.

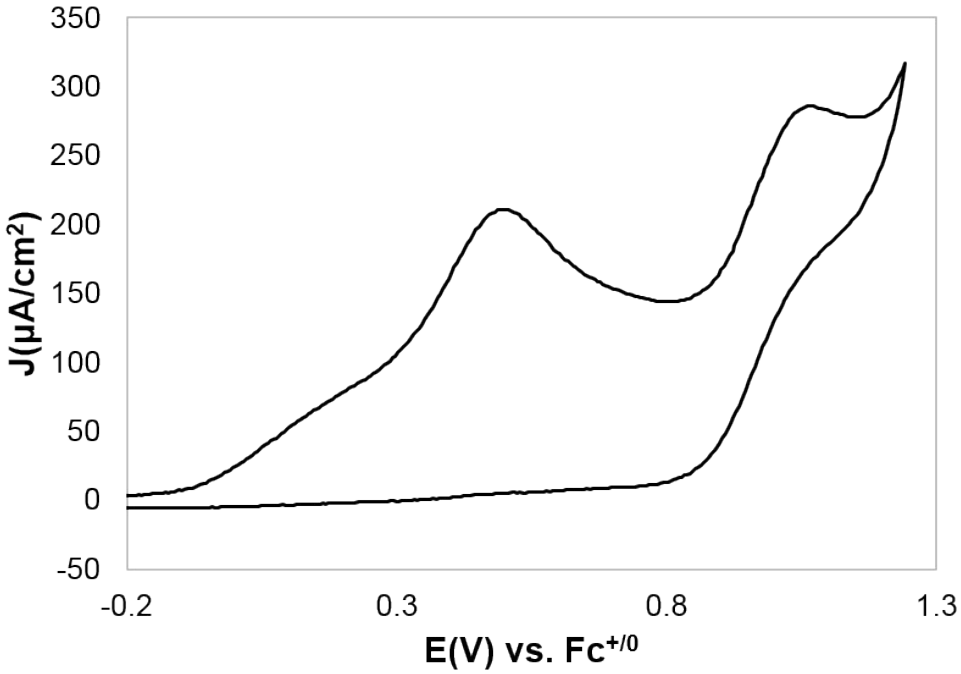


Figure S8. Cyclic voltammogram of **3** under N_2 in THF with 0.1 M [nBu$_4$N][PF$_6$] as the supporting electrolyte (scan rate: 100mV s^{-1}). Two irreversible oxidative features are observed.

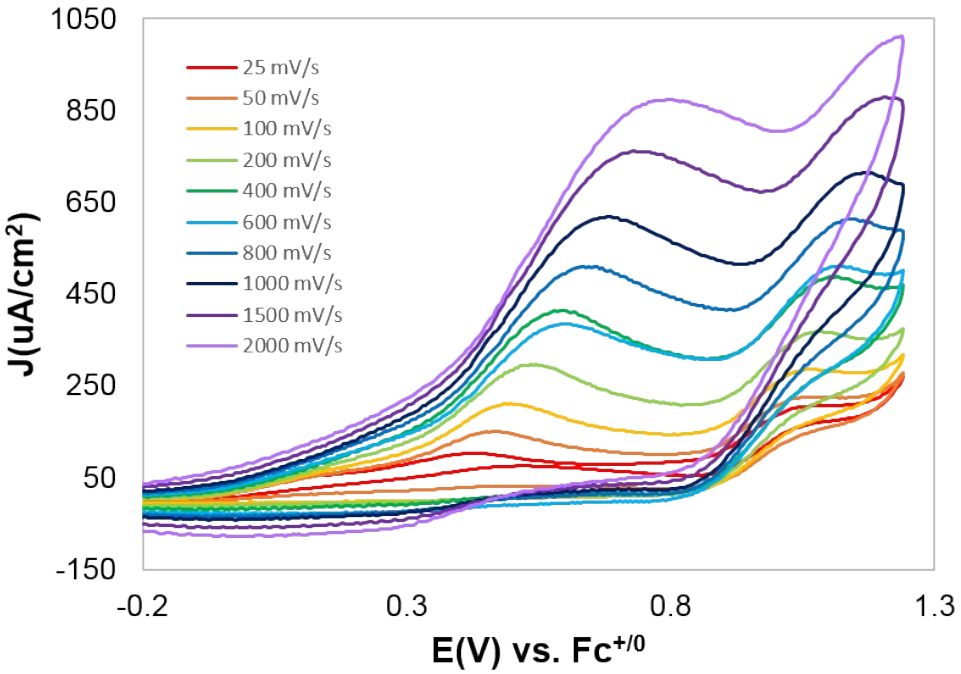


Figure S9. Cyclic voltammogram scan rate dependence of **3** in a THF solution containing 0.1 M [nBu$_4$N][PF$_6$] under an atmosphere of N_2 displaying the observed irreversible features. Scan rates vary from 25 to 2000 mV/s.

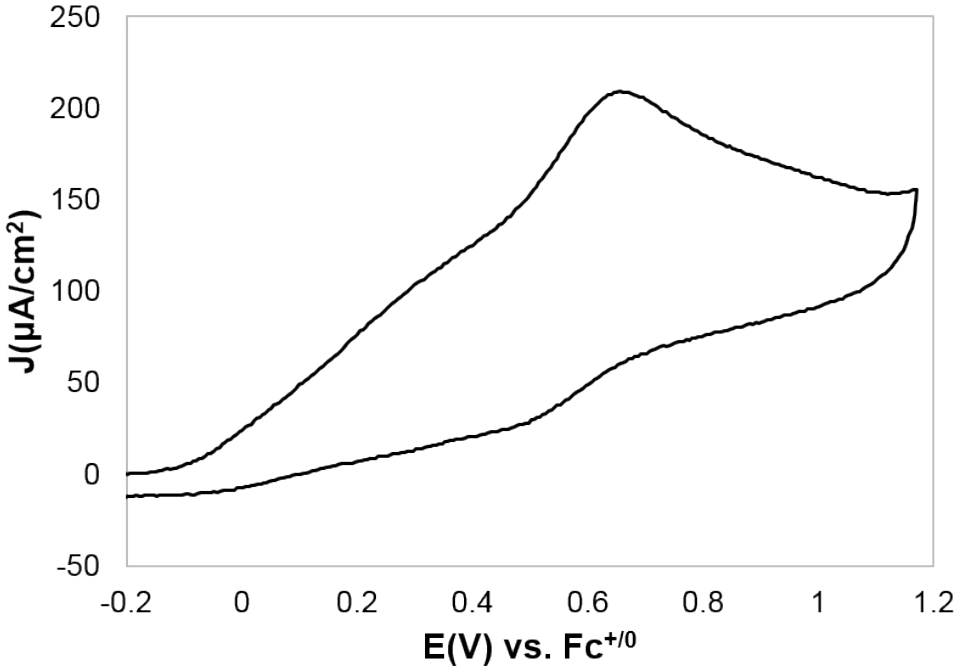


Figure S10. Cyclic voltammogram of **4** under N_2 in THF with 0.1 M [nBu$_4$N][PF$_6$] as the supporting electrolyte (scan rate: 100mV s^{-1}). One irreversible oxidative feature is observed, but the electrode is passivated with subsequent scans.

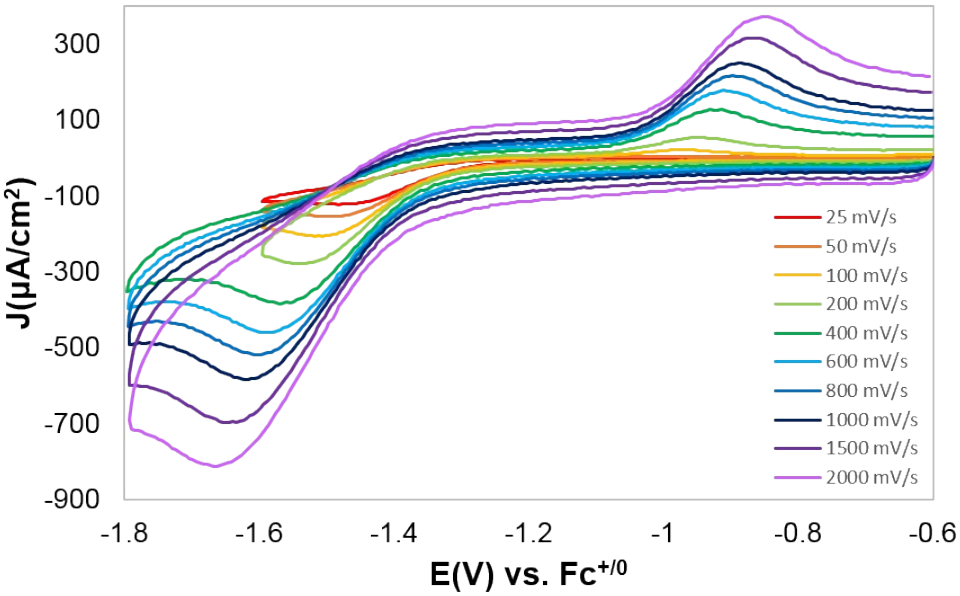


Figure S11. Cyclic voltammogram scan rate dependence of **4** in a DCM solution containing 0.1 M [nBu$_4$N][PF$_6$] under an atmosphere of N_2 displaying the observed redox couple. Scan rates vary from 25 to 2000 mV/s.

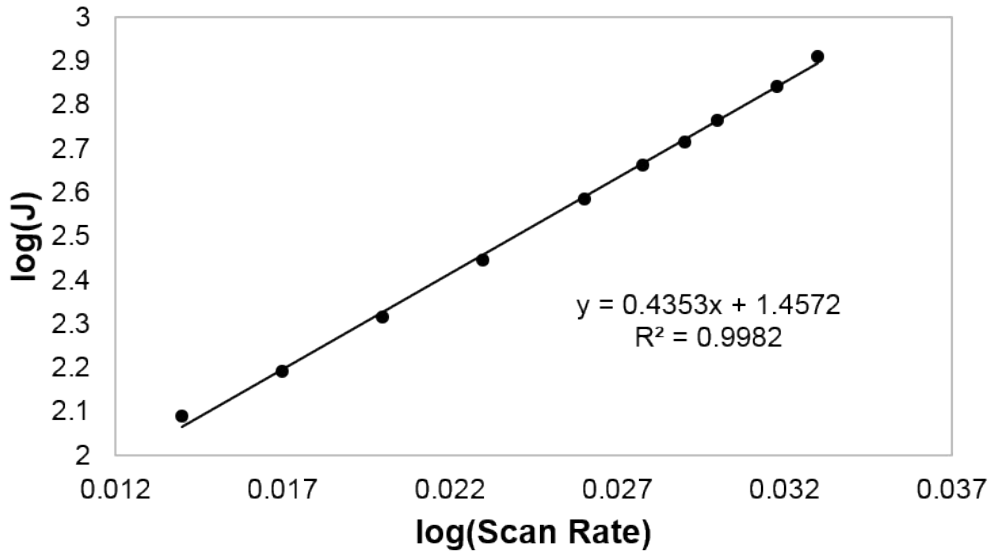


Figure S12. Plot of log(current density) versus log(scan rate). The linear relationship with a slope of approximately 0.5 indicates a diffusing molecular species rather than a species adsorbed on the electrode surface.

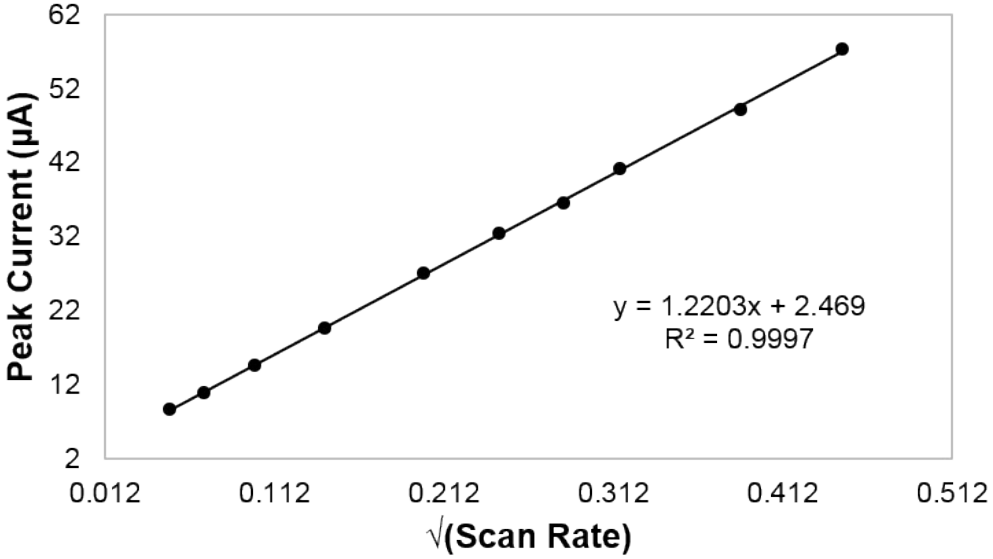


Figure S13. Plot of peak current versus the square root of the scan rate. The linear relationship indicates a freely diffusing species contributing to the observed electrochemical event.

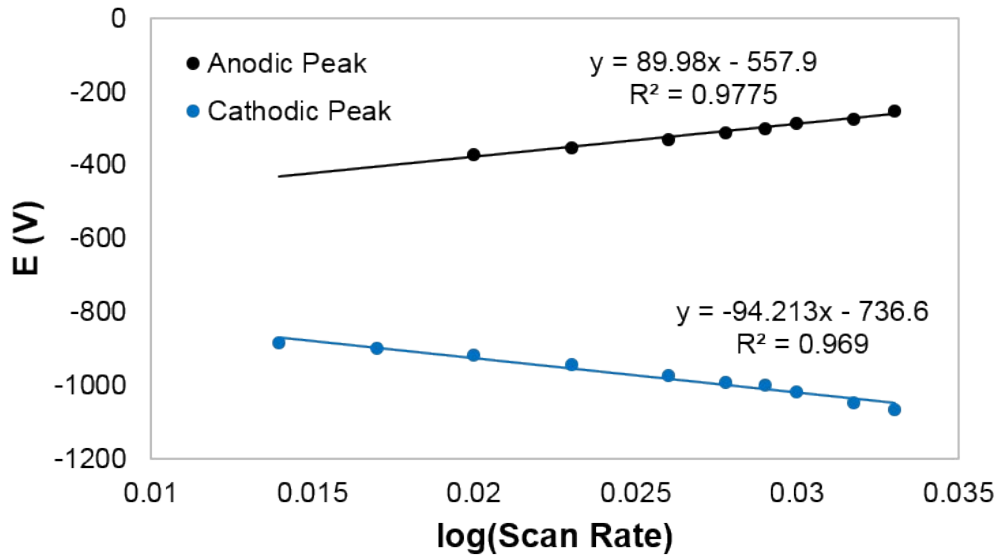


Figure S14. Laviron "trumpet" plot showing how the potential of the peak current changes as a function of scan rate for both the anodic and cathodic waves. The potential of the anodic peak shifts positively and the potential of the cathodic peak shifts negatively with increasing scan rates.

Crystal Structure of 2

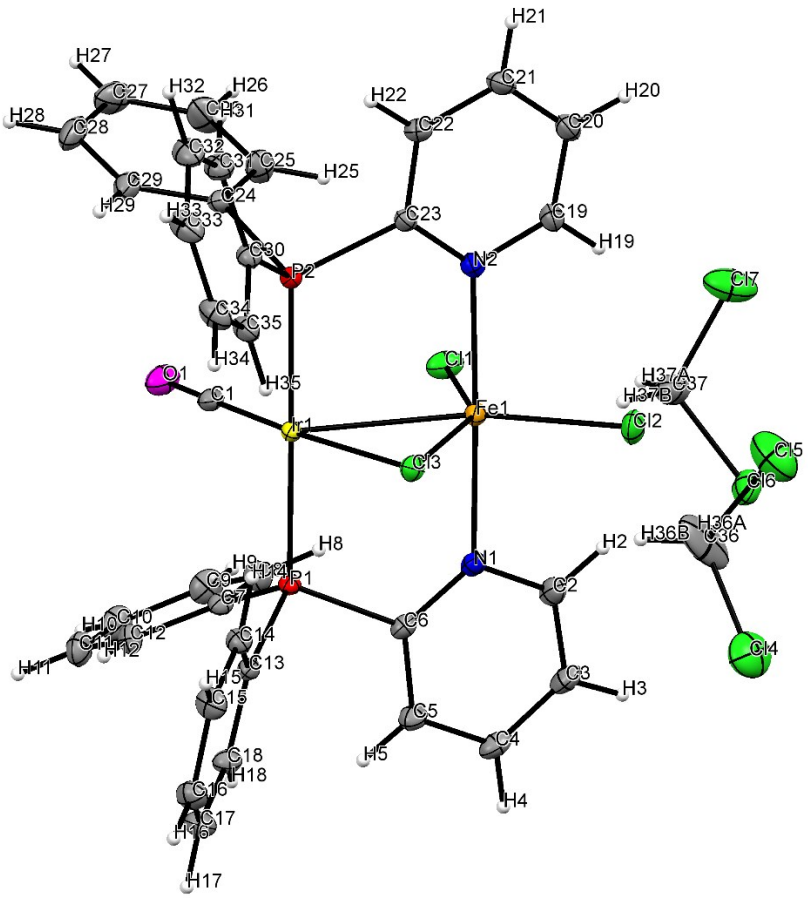


Figure S15. Molecular structure of **2** shown with 50% probability ellipsoids.

An orange prism-like specimen of $C_{37}H_{32}Cl_7FeIrN_2OP_2$, approximate dimensions 0.050 mm x 0.050 mm x 0.122 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX DUO system equipped with a fine-focus tube (MoKα, λ = 0.71073 Å) and a TRIUMPH curved-crystal monochromator.

The frames were integrated with the Bruker SAINT software package using a SAINT V8.38A (Bruker AXS, 2013) algorithm. The integration of the data using a monoclinic unit cell yielded a total of 99986 reflections to a maximum θ angle of 31.55° (0.68 Å resolution), of which 12805 were independent (average redundancy 7.808, completeness = 95.4%, R_{int} = 4.17%, R_{sig} = 2.50%) and 11585 (90.47%) were greater than $2\sigma(F^2)$. The final cell constants of a = 9.706(3) Å, b = 16.933(4) Å, c = 24.815(6) Å, β = 100.009(4)°, volume = 4016.3(18) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). Data were corrected for absorption effects using the multi-scan method (SADABS).

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/n 1, with Z = 4 for the formula unit, $C_{37}H_{32}Cl_7FeIrN_2OP_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 509 variables converged at R1 = 2.36%, for the observed data and wR2 = 5.86% for all data. The goodness-of-fit was 1.043. The largest peak in the final difference electron density synthesis was 0.792 $e^-/Å^3$ and the largest hole was -1.041 $e^-/Å^3$ with an RMS deviation of 0.105 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.784 g/cm^3 and F(000), 2112 e^-.

Table S2. Sample and crystal data for **2**.

Identification code	IrFe	
Chemical formula	$C_{37}H_{32}Cl_7FeIrN_2OP_2$	
Formula weight	1078.78 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.050 x 0.050 x 0.122 mm	
Crystal habit	orange prism	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 9.706(3) Å	α = 90°
	b = 16.933(4) Å	β = 100.009(4)°
	c = 24.815(6) Å	γ = 90°
Volume	4016.3(18) $Å^3$	
Z	4	
Density (calculated)	1.784 g/cm^3	
Absorption coefficient	4.250 mm^{-1}	
F(000)	2112	

Table S3. Data collection and structure refinement for **2**.

Diffractometer	Bruker APEX DUO	
Radiation source	fine-focus tube (MoKα , λ = 0.71073 Å)	
Theta range for data collection	1.46 to 31.55°	
Index ranges	-14<=h<=14, -23<=k<=24, -36<=l<=36	
Reflections collected	99986	
Independent reflections	12805 [R(int) = 0.0417]	
Absorption correction	multi-scan	
Structure solution technique	direct methods	
Structure solution program	SHELXTL XT 2014/5 (Bruker AXS, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXTL XL 2017/1 (Bruker AXS, 2017)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	12805 / 13 / 509	
Goodness-of-fit on F^2	1.043	
Δ/σ_{max}	0.001	
Final R indices	11585 data; I>2σ(I)	R1 = 0.0236, wR2 = 0.0570
	all data	R1 = 0.0286, wR2 = 0.0586
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0243P)^2+7.1070P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	0.792 and -1.041 $eÅ^{-3}$	
R.M.S. deviation from mean	0.105 $eÅ^{-3}$	

Table S4. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for **2**.

	x/a	**y/b**	**z/c**	**U(eq)**

	x/a	y/b	z/c	U(eq)
C1	0.7901(2)	0.62978(13)	0.44865(9)	0.0136(4)
C2	0.5266(2)	0.48763(15)	0.25016(10)	0.0184(4)
C3	0.5031(3)	0.40828(15)	0.24003(10)	0.0200(5)
C4	0.5939(3)	0.35351(14)	0.26874(10)	0.0189(5)
C5	0.7021(3)	0.38165(14)	0.30838(10)	0.0167(4)
C6	0.7172(2)	0.46272(13)	0.31755(9)	0.0126(4)
C7	0.7781(2)	0.45005(13)	0.43172(9)	0.0119(4)
C8	0.6337(2)	0.45087(15)	0.43132(10)	0.0175(4)
C9	0.5792(3)	0.41599(16)	0.47391(10)	0.0208(5)
C10	0.6682(3)	0.38128(16)	0.51748(10)	0.0214(5)
C11	0.8115(3)	0.38184(16)	0.51836(10)	0.0208(5)
C12	0.8671(2)	0.41651(14)	0.47585(9)	0.0161(4)
C13	0.0111(2)	0.45340(13)	0.37199(9)	0.0116(4)
C14	0.1218(2)	0.50126(14)	0.36250(9)	0.0148(4)
C15	0.2500(2)	0.46842(15)	0.35696(11)	0.0189(5)
C16	0.2696(3)	0.38717(15)	0.36125(11)	0.0197(5)
C17	0.1604(3)	0.33880(14)	0.37158(10)	0.0182(4)
C18	0.0325(2)	0.37136(13)	0.37746(10)	0.0150(4)
C19	0.5377(2)	0.81871(14)	0.27151(9)	0.0161(4)
C20	0.5292(3)	0.90034(14)	0.26734(10)	0.0177(4)
C21	0.6320(3)	0.94593(14)	0.29841(10)	0.0188(5)
C22	0.7368(2)	0.90764(14)	0.33437(9)	0.0161(4)
C23	0.7370(2)	0.82528(13)	0.33735(9)	0.0125(4)
C24	0.7971(2)	0.80851(13)	0.45253(9)	0.0151(4)
C25	0.6534(3)	0.81628(17)	0.45150(10)	0.0223(5)
C26	0.6030(3)	0.83636(19)	0.49870(12)	0.0307(6)
C27	0.6959(4)	0.84889(17)	0.54726(12)	0.0307(6)
C28	0.8385(3)	0.84040(17)	0.54889(11)	0.0281(6)
C29	0.8895(3)	0.81938(15)	0.50163(10)	0.0202(5)
C30	0.0283(2)	0.82080(13)	0.39370(9)	0.0135(4)
C31	0.0554(2)	0.89752(14)	0.41475(10)	0.0181(4)
C32	0.1852(3)	0.93246(15)	0.41540(11)	0.0222(5)
C33	0.2903(3)	0.89119(16)	0.39544(12)	0.0235(5)
C34	0.2653(2)	0.81525(15)	0.37503(11)	0.0202(5)
C35	0.1346(2)	0.78032(14)	0.37436(10)	0.0164(4)
Cl1	0.45530(6)	0.64322(3)	0.34725(3)	0.01989(11)
Cl2	0.56907(6)	0.66240(4)	0.19969(2)	0.02142(11)
Cl3	0.90013(6)	0.64590(3)	0.29233(2)	0.01370(9)
Fe1	0.63379(3)	0.64856(2)	0.29558(2)	0.01168(6)
Ir1	0.85233(2)	0.63678(2)	0.38305(2)	0.00924(3)
N1	0.6320(2)	0.51592(11)	0.28808(8)	0.0139(3)
N2	0.6403(2)	0.78060(11)	0.30518(8)	0.0133(3)
O1	0.7479(2)	0.62533(11)	0.48877(7)	0.0218(4)
P1	0.84410(6)	0.49980(3)	0.37624(2)	0.01023(10)

	x/a	y/b	z/c	U(eq)
P2	0.85848(6)	0.77352(3)	0.39134(2)	0.01056(10)
C36	0.802(3)	0.6328(7)	0.1087(5)	0.057(6)
Cl4	0.8248(8)	0.5504(3)	0.0677(3)	0.0426(12)
Cl5	0.7777(6)	0.7203(4)	0.0706(4)	0.0465(12)
C36A	0.820(2)	0.6338(6)	0.1103(5)	0.029(3)
Cl4A	0.777(3)	0.5564(5)	0.0611(3)	0.071(3)
Cl5A	0.8032(18)	0.7270(5)	0.0785(5)	0.0519(19)
C37	0.2065(12)	0.6221(4)	0.2333(4)	0.0260(14)
Cl6	0.1751(8)	0.5479(3)	0.1825(4)	0.0251(5)
Cl7	0.1587(6)	0.71769(11)	0.2083(2)	0.0381(7)
C37A	0.214(4)	0.6388(10)	0.2305(12)	0.0260(14)
Cl6A	0.1763(13)	0.5495(6)	0.1950(3)	0.0251(5)
Cl7A	0.1164(19)	0.7146(4)	0.1923(8)	0.0381(7)
C37B	0.195(3)	0.6458(16)	0.2138(14)	0.0260(14)
Cl6B	0.188(4)	0.5518(15)	0.182(2)	0.0251(5)
Cl7B	0.0735(18)	0.7090(5)	0.1744(8)	0.0381(7)

Table S5. Bond lengths (Å) for **2**.

C1-O1	1.143(3)	C1-Ir1	1.836(2)
C2-N1	1.352(3)	C2-C3	1.379(3)
C2-H2	0.95	C3-C4	1.388(4)
C3-H3	0.95	C4-C5	1.392(3)
C4-H4	0.95	C5-C6	1.395(3)
C5-H5	0.95	C6-N1	1.349(3)
C6-P1	1.846(2)	C7-C12	1.392(3)
C7-C8	1.400(3)	C7-P1	1.823(2)
C8-C9	1.393(3)	C8-H8	0.95
C9-C10	1.391(4)	C9-H9	0.95
C10-C11	1.387(4)	C10-H10	0.95
C11-C12	1.395(3)	C11-H11	0.95
C12-H12	0.95	C13-C14	1.399(3)
C13-C18	1.408(3)	C13-P1	1.821(2)
C14-C15	1.391(3)	C14-H14	0.95
C15-C16	1.390(4)	C15-H15	0.95
C16-C17	1.398(3)	C16-H16	0.95
C17-C18	1.389(3)	C17-H17	0.95
C18-H18	0.95	C19-N2	1.348(3)
C19-C20	1.388(3)	C19-H19	0.95
C20-C21	1.385(4)	C20-H20	0.95
C21-C22	1.391(3)	C21-H21	0.95
C22-C23	1.397(3)	C22-H22	0.95
C23-N2	1.353(3)	C23-P2	1.845(2)
C24-C29	1.394(3)	C24-C25	1.397(3)
C24-P2	1.823(2)	C25-C26	1.388(3)

C25-H25	0.95	C26-C27	1.390(5)
C26-H26	0.95	C27-C28	1.385(5)
C27-H27	0.95	C28-C29	1.396(4)
C28-H28	0.95	C29-H29	0.95
C30-C35	1.392(3)	C30-C31	1.408(3)
C30-P2	1.824(2)	C31-C32	1.390(3)
C31-H31	0.95	C32-C33	1.396(4)
C32-H32	0.95	C33-C34	1.388(4)
C33-H33	0.95	C34-C35	1.397(3)
C34-H34	0.95	C35-H35	0.95
Cl1-Fe1	2.3293(8)	Cl2-Fe1	2.3648(9)
Cl3-Ir1	2.3814(8)	Cl3-Fe1	2.6007(9)
Fe1-N2	2.248(2)	Fe1-N1	2.254(2)
Fe1-Ir1	2.7660(6)	Ir1-P2	2.3243(8)
Ir1-P1	2.3261(8)	C36-Cl5	1.753(10)
C36-Cl4	1.763(11)	C36-H36A	0.99
C36-H36B	0.99	C36A-Cl5A	1.761(10)
C36A-Cl4A	1.792(10)	C36A-H36C	0.99
C36A-H36D	0.99	C37-Cl7	1.766(6)
C37-Cl6	1.770(7)	C37-H37A	0.99
C37-H37B	0.99	C37A-Cl6A	1.756(15)
C37A-Cl7A	1.771(16)	C37A-H37C	0.99
C37A-H37D	0.99	C37B-Cl7B	1.758(17)
C37B-Cl6B	1.770(16)	C37B-H37E	0.99
C37B-H37F	0.99		

Table S6. Bond angles (°) for **2**.

O1-C1-Ir1	178.2(2)	N1-C2-C3	123.6(2)
N1-C2-H2	118.2	C3-C2-H2	118.2
C2-C3-C4	119.1(2)	C2-C3-H3	120.4
C4-C3-H3	120.4	C3-C4-C5	117.9(2)
C3-C4-H4	121.0	C5-C4-H4	121.0
C4-C5-C6	119.8(2)	C4-C5-H5	120.1
C6-C5-H5	120.1	N1-C6-C5	122.1(2)
N1-C6-P1	117.55(16)	C5-C6-P1	120.01(18)
C12-C7-C8	119.5(2)	C12-C7-P1	122.11(17)
C8-C7-P1	118.21(17)	C9-C8-C7	120.2(2)
C9-C8-H8	119.9	C7-C8-H8	119.9
C10-C9-C8	120.1(2)	C10-C9-H9	119.9
C8-C9-H9	119.9	C11-C10-C9	119.7(2)
C11-C10-H10	120.2	C9-C10-H10	120.2
C10-C11-C12	120.6(2)	C10-C11-H11	119.7
C12-C11-H11	119.7	C7-C12-C11	119.9(2)

C7-C12-H12	120.1	C11-C12-H12	120.1
C14-C13-C18	118.9(2)	C14-C13-P1	118.54(17)
C18-C13-P1	122.55(17)	C15-C14-C13	120.8(2)
C15-C14-H14	119.6	C13-C14-H14	119.6
C16-C15-C14	120.1(2)	C16-C15-H15	120.0
C14-C15-H15	120.0	C15-C16-C17	119.7(2)
C15-C16-H16	120.2	C17-C16-H16	120.2
C18-C17-C16	120.5(2)	C18-C17-H17	119.8
C16-C17-H17	119.8	C17-C18-C13	120.1(2)
C17-C18-H18	120.0	C13-C18-H18	120.0
N2-C19-C20	123.5(2)	N2-C19-H19	118.3
C20-C19-H19	118.3	C21-C20-C19	119.0(2)
C21-C20-H20	120.5	C19-C20-H20	120.5
C20-C21-C22	118.2(2)	C20-C21-H21	120.9
C22-C21-H21	120.9	C21-C22-C23	119.6(2)
C21-C22-H22	120.2	C23-C22-H22	120.2
N2-C23-C22	122.2(2)	N2-C23-P2	116.94(16)
C22-C23-P2	120.50(17)	C29-C24-C25	119.5(2)
C29-C24-P2	121.15(19)	C25-C24-P2	119.01(18)
C26-C25-C24	120.3(3)	C26-C25-H25	119.8
C24-C25-H25	119.8	C25-C26-C27	119.9(3)
C25-C26-H26	120.1	C27-C26-H26	120.1
C28-C27-C26	120.3(2)	C28-C27-H27	119.9
C26-C27-H27	119.9	C27-C28-C29	120.0(3)
C27-C28-H28	120.0	C29-C28-H28	120.0
C24-C29-C28	120.0(3)	C24-C29-H29	120.0
C28-C29-H29	120.0	C35-C30-C31	118.7(2)
C35-C30-P2	119.52(17)	C31-C30-P2	121.76(17)
C32-C31-C30	120.5(2)	C32-C31-H31	119.7
C30-C31-H31	119.7	C31-C32-C33	120.0(2)
C31-C32-H32	120.0	C33-C32-H32	120.0
C34-C33-C32	120.1(2)	C34-C33-H33	120.0
C32-C33-H33	120.0	C33-C34-C35	119.8(2)
C33-C34-H34	120.1	C35-C34-H34	120.1
C30-C35-C34	120.9(2)	C30-C35-H35	119.6
C34-C35-H35	119.6	Ir1-Cl3-Fe1	67.280(16)
N2-Fe1-N1	178.37(7)	N2-Fe1-Cl1	89.44(5)
N1-Fe1-Cl1	90.63(5)	N2-Fe1-Cl2	90.33(5)
N1-Fe1-Cl2	91.07(5)	Cl1-Fe1-Cl2	117.70(3)
N2-Fe1-Cl3	90.61(5)	N1-Fe1-Cl3	88.48(5)
Cl1-Fe1-Cl3	148.74(3)	Cl2-Fe1-Cl3	93.56(2)
N2-Fe1-Ir1	89.14(5)	N1-Fe1-Ir1	89.24(5)
Cl1-Fe1-Ir1	96.17(3)	Cl2-Fe1-Ir1	146.12(2)
Cl3-Fe1-Ir1	52.574(19)	C1-Ir1-P2	89.61(7)
C1-Ir1-P1	89.29(7)	P2-Ir1-P1	178.897(19)

C1-Ir1-Cl3	172.16(7)	P2-Ir1-Cl3	90.735(19)
P1-Ir1-Cl3	90.329(18)	C1-Ir1-Fe1	112.03(7)
P2-Ir1-Fe1	90.112(15)	P1-Ir1-Fe1	90.166(15)
Cl3-Ir1-Fe1	60.15(2)	C6-N1-C2	117.3(2)
C6-N1-Fe1	128.73(15)	C2-N1-Fe1	113.87(16)
C19-N2-C23	117.4(2)	C19-N2-Fe1	113.98(15)
C23-N2-Fe1	128.52(15)	C13-P1-C7	106.11(10)
C13-P1-C6	106.63(10)	C7-P1-C6	99.49(10)
C13-P1-Ir1	114.51(7)	C7-P1-Ir1	114.71(7)
C6-P1-Ir1	113.97(7)	C24-P2-C30	104.75(11)
C24-P2-C23	100.97(10)	C30-P2-C23	105.95(10)
C24-P2-Ir1	112.97(8)	C30-P2-Ir1	116.69(8)
C23-P2-Ir1	113.93(7)	Cl5-C36-Cl4	112.1(7)
Cl5-C36-H36A	109.2	Cl4-C36-H36A	109.2
Cl5-C36-H36B	109.2	Cl4-C36-H36B	109.2
H36A-C36-H36B	107.9	Cl5A-C36A-Cl4A	111.0(7)
Cl5A-C36A-H36C	109.4	Cl4A-C36A-H36C	109.4
Cl5A-C36A-H36D	109.4	Cl4A-C36A-H36D	109.4
H36C-C36A-H36D	108.0	Cl7-C37-Cl6	113.5(5)
Cl7-C37-H37A	108.9	Cl6-C37-H37A	108.9
Cl7-C37-H37B	108.9	Cl6-C37-H37B	108.9
H37A-C37-H37B	107.7	Cl6A-C37A-Cl7A	108.1(11)
Cl6A-C37A-H37C	110.1	Cl7A-C37A-H37C	110.1
Cl6A-C37A-H37D	110.1	Cl7A-C37A-H37D	110.1
H37C-C37A-H37D	108.4	Cl7B-C37B-Cl6B	109.2(17)
Cl7B-C37B-H37E	109.8	Cl6B-C37B-H37E	109.8
Cl7B-C37B-H37F	109.8	Cl6B-C37B-H37F	109.8
H37E-C37B-H37F	108.3		

Table S7. Torsion angles (°) for **2**.

N1-C2-C3-C4	-2.1(4)	C2-C3-C4-C5	2.7(4)
C3-C4-C5-C6	-0.8(4)	C4-C5-C6-N1	-1.8(3)
C4-C5-C6-P1	171.43(18)	C12-C7-C8-C9	-2.1(4)
P1-C7-C8-C9	-177.75(19)	C7-C8-C9-C10	1.0(4)
C8-C9-C10-C11	0.2(4)	C9-C10-C11-C12	-0.3(4)
C8-C7-C12-C11	2.0(3)	P1-C7-C12-C11	177.46(19)
C10-C11-C12-C7	-0.8(4)	C18-C13-C14-C15	1.8(3)
P1-C13-C14-C15	-177.69(18)	C13-C14-C15-C16	-0.5(4)
C14-C15-C16-C17	-0.5(4)	C15-C16-C17-C18	0.1(4)
C16-C17-C18-C13	1.2(4)	C14-C13-C18-C17	-2.2(3)
P1-C13-C18-C17	177.31(18)	N2-C19-C20-C21	1.2(4)
C19-C20-C21-C22	-2.7(3)	C20-C21-C22-C23	1.2(3)
C21-C22-C23-N2	1.9(3)	C21-C22-C23-P2	-171.08(18)
C29-C24-C25-C26	1.4(4)	P2-C24-C25-C26	174.6(2)
C24-C25-C26-C27	0.1(5)	C25-C26-C27-C28	-0.8(5)

C26-C27-C28-C29	0.2(4)	C25-C24-C29-C28	-2.1(4)
P2-C24-C29-C28	-175.1(2)	C27-C28-C29-C24	1.3(4)
C35-C30-C31-C32	1.0(4)	P2-C30-C31-C32	-179.17(19)
C30-C31-C32-C33	-0.5(4)	C31-C32-C33-C34	-0.1(4)
C32-C33-C34-C35	0.2(4)	C31-C30-C35-C34	-0.9(3)
P2-C30-C35-C34	179.25(19)	C33-C34-C35-C30	0.3(4)
C5-C6-N1-C2	2.5(3)	P1-C6-N1-C2	-170.93(17)
C5-C6-N1-Fe1	179.33(16)	P1-C6-N1-Fe1	5.9(3)
C3-C2-N1-C6	-0.5(4)	C3-C2-N1-Fe1	-177.8(2)
C20-C19-N2-C23	1.8(3)	C20-C19-N2-Fe1	-174.34(18)
C22-C23-N2-C19	-3.4(3)	P2-C23-N2-C19	169.84(16)
C22-C23-N2-Fe1	172.15(16)	P2-C23-N2-Fe1	-14.6(3)
C14-C13-P1-C7	-139.71(18)	C18-C13-P1-C7	40.8(2)
C14-C13-P1-C6	114.90(18)	C18-C13-P1-C6	-64.6(2)
C14-C13-P1-Ir1	-12.1(2)	C18-C13-P1-Ir1	168.39(16)
C12-C7-P1-C13	28.6(2)	C8-C7-P1-C13	-155.93(18)
C12-C7-P1-C6	139.10(19)	C8-C7-P1-C6	-45.4(2)
C12-C7-P1-Ir1	-98.87(19)	C8-C7-P1-Ir1	76.61(19)
N1-C6-P1-C13	-134.20(17)	C5-C6-P1-C13	52.3(2)
N1-C6-P1-C7	115.71(18)	C5-C6-P1-C7	-57.8(2)
N1-C6-P1-Ir1	-6.85(19)	C5-C6-P1-Ir1	179.60(16)
C29-C24-P2-C30	-37.3(2)	C25-C24-P2-C30	149.6(2)
C29-C24-P2-C23	-147.2(2)	C25-C24-P2-C23	39.7(2)
C29-C24-P2-Ir1	90.7(2)	C25-C24-P2-Ir1	-82.3(2)
C35-C30-P2-C24	145.16(19)	C31-C30-P2-C24	-34.7(2)
C35-C30-P2-C23	-108.59(19)	C31-C30-P2-C23	71.5(2)
C35-C30-P2-Ir1	19.4(2)	C31-C30-P2-Ir1	-160.45(17)
N2-C23-P2-C24	-109.61(18)	C22-C23-P2-C24	63.7(2)
N2-C23-P2-C30	141.42(17)	C22-C23-P2-C30	-45.3(2)
N2-C23-P2-Ir1	11.78(19)	C22-C23-P2-Ir1	-174.89(16)

Table S8. Anisotropic atomic displacement parameters (Å^2) for **2**.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0157(10)	0.0104(9)	0.0149(10)	-0.0015(8)	0.0031(8)	0.0001(7)
C2	0.0131(10)	0.0209(11)	0.0198(11)	-0.0055(9)	-0.0010(8)	0.0023(8)
C3	0.0175(11)	0.0219(12)	0.0201(11)	-0.0094(9)	0.0022(9)	-0.0042(9)
C4	0.0225(12)	0.0158(11)	0.0196(11)	-0.0060(9)	0.0068(9)	-0.0059(9)
C5	0.0204(11)	0.0135(10)	0.0163(10)	-0.0007(8)	0.0032(8)	-0.0028(8)
C6	0.0131(9)	0.0131(10)	0.0121(9)	-0.0027(7)	0.0039(7)	-0.0026(7)
C7	0.0138(9)	0.0102(9)	0.0121(9)	0.0003(7)	0.0037(7)	-0.0020(7)
C8	0.0143(10)	0.0202(11)	0.0182(11)	0.0012(9)	0.0035(8)	-0.0001(8)
C9	0.0183(11)	0.0257(12)	0.0207(11)	-0.0022(10)	0.0097(9)	-0.0047(9)
C10	0.0259(12)	0.0241(12)	0.0164(11)	0.0009(9)	0.0094(9)	-0.0053(10)
C11	0.0254(12)	0.0237(12)	0.0130(10)	0.0028(9)	0.0020(9)	-0.0021(9)

C12	0.0169(10)	0.0178(10)	0.0133(10)	0.0022(8)	0.0017(8)	0.0002(8)
C13	0.0129(9)	0.0112(9)	0.0106(9)	-0.0007(7)	0.0015(7)	-0.0006(7)
C14	0.0137(10)	0.0131(10)	0.0170(10)	0.0008(8)	0.0010(8)	-0.0016(8)
C15	0.0116(10)	0.0199(11)	0.0250(12)	0.0006(9)	0.0026(8)	-0.0027(8)
C16	0.0146(10)	0.0200(11)	0.0243(12)	-0.0015(9)	0.0031(9)	0.0026(8)
C17	0.0190(11)	0.0131(10)	0.0228(11)	0.0012(9)	0.0046(9)	0.0022(8)
C18	0.0163(10)	0.0121(10)	0.0172(10)	-0.0001(8)	0.0046(8)	-0.0007(8)
C19	0.0160(10)	0.0175(11)	0.0139(10)	0.0014(8)	0.0000(8)	0.0022(8)
C20	0.0198(11)	0.0181(11)	0.0150(10)	0.0024(8)	0.0027(8)	0.0056(8)
C21	0.0251(12)	0.0132(10)	0.0185(11)	0.0019(8)	0.0053(9)	0.0063(9)
C22	0.0197(11)	0.0116(10)	0.0167(10)	-0.0017(8)	0.0024(8)	0.0012(8)
C23	0.0146(10)	0.0123(10)	0.0110(9)	0.0005(7)	0.0032(7)	0.0023(7)
C24	0.0214(11)	0.0117(10)	0.0130(10)	-0.0002(8)	0.0047(8)	0.0019(8)
C25	0.0225(12)	0.0303(13)	0.0152(11)	0.0006(10)	0.0060(9)	0.0067(10)
C26	0.0344(15)	0.0378(16)	0.0235(13)	0.0033(12)	0.0155(11)	0.0135(12)
C27	0.0501(18)	0.0266(14)	0.0190(12)	-0.0010(10)	0.0161(12)	0.0063(12)
C28	0.0483(17)	0.0223(13)	0.0123(11)	-0.0024(9)	0.0018(11)	-0.0052(12)
C29	0.0266(12)	0.0174(11)	0.0156(11)	-0.0022(9)	0.0006(9)	-0.0028(9)
C30	0.0132(9)	0.0118(10)	0.0150(10)	0.0014(8)	0.0008(8)	-0.0015(7)
C31	0.0171(10)	0.0142(11)	0.0221(11)	-0.0004(9)	0.0011(8)	-0.0017(8)
C32	0.0204(12)	0.0147(11)	0.0292(13)	0.0002(9)	-0.0024(10)	-0.0043(9)
C33	0.0152(11)	0.0184(11)	0.0352(14)	0.0062(10)	-0.0002(10)	-0.0025(9)
C34	0.0125(10)	0.0193(11)	0.0286(13)	0.0046(10)	0.0029(9)	0.0010(8)
C35	0.0147(10)	0.0136(10)	0.0199(11)	0.0027(8)	0.0003(8)	0.0011(8)
Cl1	0.0230(3)	0.0165(3)	0.0236(3)	-0.0016(2)	0.0135(2)	-0.0024(2)
Cl2	0.0237(3)	0.0290(3)	0.0107(2)	-0.0001(2)	0.0006(2)	0.0035(2)
Cl3	0.0154(2)	0.0147(2)	0.0117(2)	0.00073(17)	0.00420(17)	0.00027(17)
Fe1	0.01198(14)	0.01291(14)	0.00993(13)	-0.00040(11)	0.00126(11)	0.00012(10)
Ir1	0.00973(4)	0.00896(4)	0.00900(4)	0.00002(3)	0.00158(3)	-0.00011(3)
N1	0.0133(8)	0.0146(9)	0.0140(8)	-0.0035(7)	0.0028(7)	0.0006(7)
N2	0.0130(8)	0.0143(9)	0.0126(8)	0.0010(7)	0.0024(7)	0.0011(7)
O1	0.0295(10)	0.0197(9)	0.0187(8)	-0.0011(7)	0.0114(7)	-0.0028(7)
P1	0.0113(2)	0.0093(2)	0.0102(2)	0.00014(18)	0.00213(18)	-0.00089(18)
P2	0.0113(2)	0.0100(2)	0.0101(2)	-0.00040(18)	0.00107(18)	0.00044(18)
C36	0.074(11)	0.068(10)	0.039(7)	0.039(6)	0.034(7)	0.035(7)
Cl4	0.059(3)	0.0386(13)	0.0325(16)	0.0121(10)	0.0157(13)	-0.0032(12)
Cl5	0.0341(19)	0.045(2)	0.059(3)	0.0185(15)	0.0061(15)	0.0006(12)
C36A	0.028(4)	0.028(6)	0.033(7)	-0.002(5)	0.007(4)	0.008(4)
Cl4A	0.125(9)	0.048(2)	0.0408(18)	0.0120(14)	0.014(3)	-0.012(4)
Cl5A	0.082(4)	0.0324(18)	0.049(3)	0.0148(16)	0.034(3)	0.022(2)
C37	0.0230(19)	0.024(3)	0.030(2)	-0.005(2)	0.0031(17)	0.004(3)
Cl6	0.0275(10)	0.0245(5)	0.0209(10)	-0.0007(10)	-0.0025(15)	-0.0066(5)
Cl7	0.0396(15)	0.0236(4)	0.0570(16)	0.0071(7)	0.0251(14)	0.0039(7)
C37A	0.0230(19)	0.024(3)	0.030(2)	-0.005(2)	0.0031(17)	0.004(3)
Cl6A	0.0275(10)	0.0245(5)	0.0209(10)	-0.0007(10)	-0.0025(15)	-0.0066(5)

Cl7A	0.0396(15)	0.0236(4)	0.0570(16)	0.0071(7)	0.0251(14)	0.0039(7)
C37B	0.0230(19)	0.024(3)	0.030(2)	-0.005(2)	0.0031(17)	0.004(3)
Cl6B	0.0275(10)	0.0245(5)	0.0209(10)	-0.0007(10)	-0.0025(15)	-0.0066(5)
Cl7B	0.0396(15)	0.0236(4)	0.0570(16)	0.0071(7)	0.0251(14)	0.0039(7)

Table S9. Hydrogen atomic coordinates and isotropic atomic displacement parameters ($Å^2$) for **2**.

	x/a	**y/b**	**z/c**	**U(eq)**
H2	0.4654	0.5245	0.2293	0.022
H3	0.4256	0.3913	0.2137	0.024
H4	0.5827	0.2986	0.2616	0.023
H5	0.7654	0.3457	0.3291	0.02
H8	0.5728	0.4753	0.4019	0.021
H9	0.4810	0.4159	0.4732	0.025
H10	0.6310	0.3573	0.5465	0.026
H11	0.8723	0.3584	0.5482	0.025
H12	0.9654	0.4172	0.4770	0.019
H14	1.1094	0.5569	0.3598	0.018
H15	1.3242	0.5015	0.3502	0.023
H16	1.3569	0.3646	0.3572	0.024
H17	1.1738	0.2833	0.3746	0.022
H18	0.9594	0.3382	0.3852	0.018
H19	0.4676	0.7881	0.2495	0.019
H20	0.4539	0.9246	0.2435	0.021
H21	0.6310	1.0018	0.2953	0.023
H22	0.8077	0.9373	0.3567	0.019
H25	0.5899	0.8078	0.4183	0.027
H26	0.5052	0.8415	0.4978	0.037
H27	0.6615	0.8633	0.5794	0.037
H28	0.9016	0.8489	0.5822	0.034
H29	0.9872	0.8125	0.5029	0.024
H31	0.9844	0.9256	0.4286	0.022
H32	1.2025	0.9844	0.4294	0.027
H33	1.3790	0.9151	0.3958	0.028
H34	1.3368	0.7871	0.3615	0.024
H35	1.1181	0.7282	0.3605	0.02
H36A	0.7204	0.6238	0.1268	0.069
H36B	0.8859	0.6384	0.1377	0.069
H36C	0.7575	0.6309	0.1378	0.035
H36D	0.9175	0.6267	0.1296	0.035
H37A	0.1534	0.6092	0.2628	0.031
H37B	0.3072	0.6221	0.2495	0.031
H37C	0.3154	0.6504	0.2348	0.031
H37D	0.1885	0.6350	0.2673	0.031

	x/a	y/b	z/c	U(eq)
H37E	0.1731	0.6408	0.2511	0.031
H37F	0.2905	0.6680	0.2168	0.031

Crystal Structure of 3

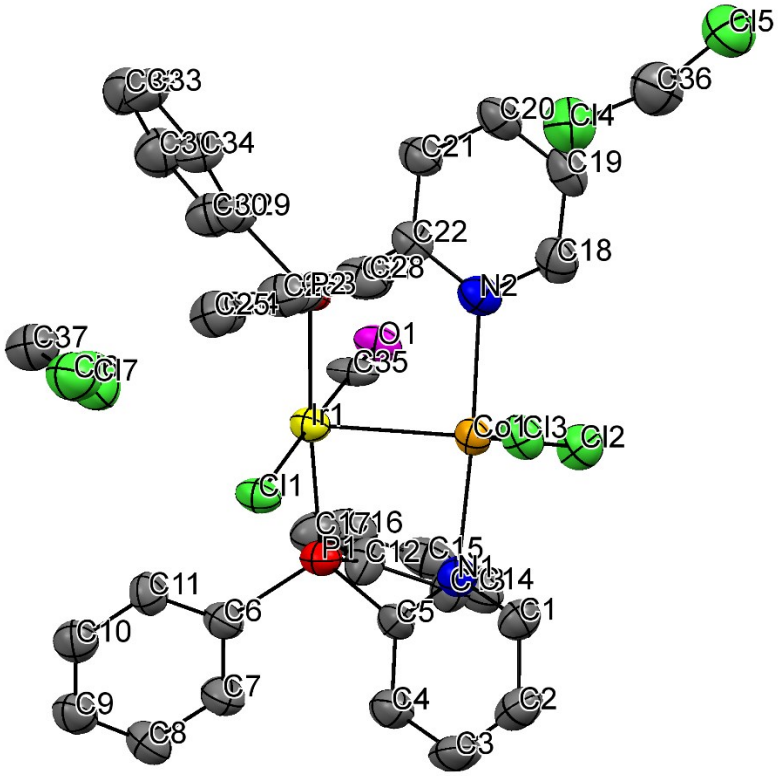


Figure S16. Molecular structure of **3** shown with 50% probability ellipsoids.

A pale green prism-like specimen of $C_{37}H_{32}Cl_7CoIrN_2OP_2$, approximate dimensions 0.390 mm x 0.494 mm x 0.497 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX II CCD system equipped with a fine-focus tube (MoKα , λ = 0.71073 Å) and a TRIUMPH curved-crystal monochromator.

The integration of the data using a monoclinic unit cell yielded a total of 30888 reflections to a maximum θ angle of 27.48° (0.77 Å resolution), of which 9186 were independent (average redundancy 3.363, completeness = 99.9%, R_{int} = 7.43%, R_{sig} = 7.89%) and 7574 (82.45%) were greater than $2\sigma(F^2)$. The final cell constants of a = 21.731(7) Å, b = 12.688(4) Å, c = 15.533(5) Å, β = 108.649(4)°, volume = 4058.(2) Å^3, are based upon the refinement of the XYZ-centroids of 9599 reflections above 20 σ(I) with 5.037° < 2θ < 55.09°. Data were corrected for absorption effects using the Numerical Mu From Formula method (SADABS). The ratio of minimum to maximum apparent transmission was 0.037. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.0001 and 0.0027.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group C 1 c 1, with Z = 4 for the formula unit, $C_{37}H_{32}Cl_7CoIrN_2OP_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 471 variables converged at R1 = 5.94%, for the observed data and wR2 = 15.36% for all data. The goodness-of-fit was 1.090. The largest peak in the final difference electron density synthesis was 3.992 e^-/Å^3 and the largest hole was -1.083 e^-/Å^3 with an RMS deviation of 0.195 e^-/Å^3. On the basis of the final model, the calculated density was 1.771 g/cm^3 and F(000), 2116 e^-.

Table S10. Sample and crystal data for **3**.

Identification code	IrCo_1	
Chemical formula	$C_{37}H_{32}Cl_7CoIrN_2OP_2$	
Formula weight	1081.86 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.390 x 0.494 x 0.497 mm	
Crystal habit	green prism	
Crystal system	monoclinic	
Space group	C 1 c 1	
Unit cell dimensions	a = 21.731(7) Å	α = 90°
	b = 12.688(4) Å	β = 108.649(4)°
	c = 15.533(5) Å	γ = 90°
Volume	4058.(2) $Å^3$	
Z	4	
Density (calculated)	1.771 g/cm^3	
Absorption coefficient	4.258 mm^{-1}	
F(000)	2116	

Table S11. Data collection and structure refinement for **3**.

Diffractometer	Bruker APEX II CCD	
Radiation source	fine-focus tube (MoKα , λ = 0.71073 Å)	
Theta range for data collection	1.89 to 27.48°	
Index ranges	-28<=h<=28, -16<=k<=16, -20<=l<=20	
Reflections collected	30888	
Independent reflections	9186 [R(int) = 0.0743]	
Coverage of independent reflections	99.9%	
Absorption correction	Numerical Mu From Formula	
Max. and min. transmission	0.0027 and 0.0001	
Structure solution technique	direct methods	
Structure solution program	SHELXTL XT 2014/5 (Bruker AXS, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXTL XL 2018/3 (Bruker AXS, 2018)	
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	9186 / 421 / 471	
Goodness-of-fit on F^2	1.090	
Final R indices	7574 data; I>2σ(I)	R1 = 0.0594, wR2 = 0.1377
	all data	R1 = 0.0786, wR2 = 0.1536
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0520P)^2+43.4173P]$ where $P=(F_o^2+2F_c^2)/3$	
Absolute structure parameter	0.040(14)	
Largest diff. peak and hole	3.992 and -1.083 $eÅ^{-3}$	
R.M.S. deviation from mean	0.195 $eÅ^{-3}$	

Table S12. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for **3**.

	x/a	y/b	z/c	U(eq)
C1	0.3712(9)	0.8609(15)	0.5973(13)	0.048(4)
C2	0.3629(11)	0.9282(16)	0.6642(14)	0.057(4)
C3	0.4134(12)	0.9840(17)	0.7162(15)	0.060(5)
C4	0.4738(10)	0.9760(15)	0.6995(13)	0.052(4)
C5	0.4788(8)	0.9089(14)	0.6325(10)	0.042(3)
C6	0.6209(8)	0.9400(12)	0.6983(11)	0.043(3)
C7	0.6267(9)	0.0453(13)	0.7275(12)	0.051(4)
C8	0.6782(9)	0.0751(15)	0.8021(12)	0.054(4)
C9	0.7244(10)	0.0012(14)	0.8462(13)	0.053(4)
C10	0.7186(9)	0.8997(14)	0.8184(12)	0.050(4)
C11	0.6679(7)	0.8679(14)	0.7446(11)	0.044(3)
C12	0.5457(9)	0.0049(14)	0.5217(14)	0.051(4)
C13	0.4862(10)	0.0618(14)	0.4810(13)	0.050(4)
C14	0.4851(11)	0.1421(16)	0.4198(14)	0.061(4)
C15	0.5394(12)	0.1652(16)	0.3952(13)	0.061(4)
C16	0.5957(13)	0.1119(17)	0.4342(15)	0.066(5)
C17	0.6001(10)	0.0337(15)	0.4964(14)	0.052(4)
C18	0.3834(10)	0.6145(16)	0.2950(12)	0.052(4)
C19	0.3838(10)	0.5458(17)	0.2250(13)	0.056(5)
C20	0.4344(10)	0.4796(16)	0.2330(12)	0.051(4)
C21	0.4859(10)	0.4859(14)	0.3126(12)	0.050(4)
C22	0.4847(8)	0.5529(13)	0.3791(11)	0.039(3)
C23	0.5299(8)	0.4530(13)	0.5526(11)	0.047(4)
C24	0.5757(10)	0.4204(13)	0.6328(11)	0.050(4)
C25	0.5611(10)	0.3396(14)	0.6843(13)	0.056(4)
C26	0.5008(9)	0.2917(15)	0.6559(13)	0.056(4)
C27	0.4540(10)	0.3271(14)	0.5770(12)	0.055(4)
C28	0.4695(9)	0.4072(13)	0.5260(12)	0.051(4)
C29	0.6199(9)	0.5136(12)	0.4569(11)	0.046(3)
C30	0.6563(10)	0.5858(16)	0.4270(15)	0.060(5)
C31	0.7073(10)	0.5529(17)	0.3982(16)	0.067(5)
C32	0.7246(11)	0.4483(17)	0.4022(16)	0.067(5)
C33	0.6890(10)	0.3751(18)	0.4324(15)	0.067(5)
C34	0.6381(10)	0.4085(14)	0.4612(15)	0.059(5)
C35	0.5516(13)	0.7780(16)	0.4333(16)	0.041(5)
O1	0.5504(8)	0.8162(13)	0.3655(12)	0.042(4)
C35A	0.550(6)	0.701(6)	0.653(4)	0.041(5)
O1A	0.548(4)	0.656(5)	0.718(3)	0.042(4)
Cl1	0.5595(3)	0.6687(4)	0.6887(4)	0.0407(16)
Cl1A	0.5589(15)	0.799(2)	0.4008(17)	0.0407(16)
Cl2	0.3728(2)	0.8532(4)	0.3677(3)	0.0520(10)

	x/a	y/b	z/c	U(eq)
Cl3	0.3597(2)	0.6206(4)	0.5177(3)	0.0464(9)
Co1	0.42801(10)	0.73405(17)	0.47614(13)	0.0352(4)
Ir1	0.55656(3)	0.73075(4)	0.54388(3)	0.03729(16)
N1	0.4288(7)	0.8495(11)	0.5835(9)	0.042(3)
N2	0.4343(7)	0.6201(12)	0.3717(10)	0.044(3)
P1	0.5530(2)	0.8991(3)	0.5998(3)	0.0394(9)
P2	0.5506(2)	0.5600(3)	0.4875(3)	0.0391(9)
C36	0.2831(12)	0.334(2)	0.2040(18)	0.078(7)
Cl4	0.3284(4)	0.2899(7)	0.3151(5)	0.093(2)
Cl5	0.2205(3)	0.2431(6)	0.1524(6)	0.0845(19)
C37	0.7798(12)	0.675(2)	0.6204(18)	0.073(6)
Cl6	0.7248(3)	0.6191(5)	0.6671(4)	0.0747(15)
Cl7	0.7542(4)	0.7927(6)	0.5628(5)	0.0870(19)

Table S13. Bond lengths (Å) for **3**.

C1-N1	1.34(2)	C1-C2	1.40(3)
C1-H1	0.95	C2-C3	1.34(3)
C2-H2	0.95	C3-C4	1.42(3)
C3-H3	0.95	C4-C5	1.38(2)
C4-H4	0.95	C5-N1	1.34(2)
C5-P1	1.843(18)	C6-C11	1.388(19)
C6-C7	1.404(19)	C6-P1	1.829(16)
C7-C8	1.382(19)	C7-H7	0.95
C8-C9	1.38(2)	C8-H8	0.95
C9-C10	1.35(2)	C9-H9	0.95
C10-C11	1.373(19)	C10-H10	0.95
C11-H11	0.95	C12-C17	1.41(3)
C12-C13	1.44(2)	C12-P1	1.782(19)
C13-C14	1.39(3)	C13-H13	0.95
C14-C15	1.38(3)	C14-H14	0.95
C15-C16	1.36(3)	C15-H15	0.95
C16-C17	1.37(3)	C16-H16	0.95
C17-H17	0.95	C18-N2	1.34(2)
C18-C19	1.40(3)	C18-H18	0.95
C19-C20	1.36(3)	C19-H19	0.95
C20-C21	1.38(3)	C20-H20	0.95
C21-C22	1.34(2)	C21-H21	0.95
C22-N2	1.37(2)	C22-P2	1.830(17)
C23-C28	1.37(2)	C23-C24	1.386(19)
C23-P2	1.833(17)	C24-C25	1.40(2)
C24-H24	0.95	C25-C26	1.38(2)
C25-H25	0.95	C26-C27	1.39(2)
C26-H26	0.95	C27-C28	1.394(19)
C27-H27	0.95	C28-H28	0.95

C29-C30	1.39(2)	C29-C34	1.387(19)
C29-P2	1.816(18)	C30-C31	1.39(2)
C30-H30	0.95	C31-C32	1.38(2)
C31-H31	0.95	C32-C33	1.38(2)
C32-H32	0.95	C33-C34	1.38(2)
C33-H33	0.95	C34-H34	0.95
C35-O1	1.15(3)	C35-Ir1	1.79(3)
C35A-O1A	1.17(4)	C35A-Ir1	1.79(4)
Cl1-Ir1	2.365(5)	Cl1A-Ir1	2.40(2)
Cl2-Co1	2.296(5)	Cl3-Co1	2.304(5)
Co1-N2	2.209(15)	Co1-N1	2.215(14)
Co1-Ir1	2.652(2)	Ir1-P1	2.316(4)
Ir1-P2	2.324(4)	C36-Cl5	1.77(2)
C36-Cl4	1.78(3)	C36-H36A	0.99
C36-H36B	0.99	C37-Cl7	1.73(3)
C37-Cl6	1.74(3)	C37-H37A	0.99
C37-H37B	0.99		

Table S14. Bond angles (°) for **3**.

N1-C1-C2	122.1(18)	N1-C1-H1	118.9
C2-C1-H1	118.9	C3-C2-C1	119.7(19)
C3-C2-H2	120.1	C1-C2-H2	120.1
C2-C3-C4	118.6(18)	C2-C3-H3	120.7
C4-C3-H3	120.7	C5-C4-C3	118.9(18)
C5-C4-H4	120.5	C3-C4-H4	120.5
N1-C5-C4	122.1(17)	N1-C5-P1	115.2(12)
C4-C5-P1	122.6(15)	C11-C6-C7	119.0(15)
C11-C6-P1	120.6(12)	C7-C6-P1	120.3(12)
C8-C7-C6	119.7(17)	C8-C7-H7	120.2
C6-C7-H7	120.2	C7-C8-C9	119.7(17)
C7-C8-H8	120.2	C9-C8-H8	120.2
C10-C9-C8	120.6(18)	C10-C9-H9	119.7
C8-C9-H9	119.7	C9-C10-C11	121.0(18)
C9-C10-H10	119.5	C11-C10-H10	119.5
C10-C11-C6	120.0(16)	C10-C11-H11	120.0
C6-C11-H11	120.0	C17-C12-C13	117.7(18)
C17-C12-P1	119.1(14)	C13-C12-P1	123.2(15)
C14-C13-C12	119.(2)	C14-C13-H13	120.5
C12-C13-H13	120.5	C15-C14-C13	121.(2)
C15-C14-H14	119.5	C13-C14-H14	119.5
C16-C15-C14	120.(2)	C16-C15-H15	120.0
C14-C15-H15	120.0	C15-C16-C17	122.(2)
C15-C16-H16	119.2	C17-C16-H16	119.2
C16-C17-C12	121.(2)	C16-C17-H17	119.6
C12-C17-H17	119.6	N2-C18-C19	121.1(18)

N2-C18-H18	119.4	C19-C18-H18	119.4
C20-C19-C18	121.4(18)	C20-C19-H19	119.3
C18-C19-H19	119.3	C19-C20-C21	116.6(18)
C19-C20-H20	121.7	C21-C20-H20	121.7
C22-C21-C20	121.0(18)	C22-C21-H21	119.5
C20-C21-H21	119.5	C21-C22-N2	122.8(16)
C21-C22-P2	122.5(14)	N2-C22-P2	114.7(12)
C28-C23-C24	119.2(16)	C28-C23-P2	121.8(12)
C24-C23-P2	118.9(13)	C23-C24-C25	120.2(18)
C23-C24-H24	119.9	C25-C24-H24	119.9
C26-C25-C24	120.4(18)	C26-C25-H25	119.8
C24-C25-H25	119.8	C25-C26-C27	119.3(18)
C25-C26-H26	120.3	C27-C26-H26	120.3
C26-C27-C28	119.6(19)	C26-C27-H27	120.2
C28-C27-H27	120.2	C23-C28-C27	121.3(17)
C23-C28-H28	119.3	C27-C28-H28	119.3
C30-C29-C34	117.8(17)	C30-C29-P2	118.9(13)
C34-C29-P2	123.2(14)	C29-C30-C31	120.7(19)
C29-C30-H30	119.6	C31-C30-H30	119.6
C32-C31-C30	121.(2)	C32-C31-H31	119.7
C30-C31-H31	119.7	C31-C32-C33	119.(2)
C31-C32-H32	120.3	C33-C32-H32	120.3
C32-C33-C34	120.(2)	C32-C33-H33	120.2
C34-C33-H33	120.2	C33-C34-C29	122.(2)
C33-C34-H34	119.2	C29-C34-H34	119.2
O1-C35-Ir1	174.3(18)	O1A-C35A-Ir1	162.(7)
N2-Co1-N1	176.2(5)	N2-Co1-Cl2	91.9(4)
N1-Co1-Cl2	89.6(4)	N2-Co1-Cl3	89.6(4)
N1-Co1-Cl3	93.0(4)	Cl2-Co1-Cl3	112.63(19)
N2-Co1-Ir1	88.7(4)	N1-Co1-Ir1	87.6(4)
Cl2-Co1-Ir1	122.58(16)	Cl3-Co1-Ir1	124.79(14)
C35A-Ir1-P1	79.(3)	C35-Ir1-P1	93.0(6)
C35A-Ir1-P2	99.(3)	C35-Ir1-P2	88.4(6)
P1-Ir1-P2	174.86(18)	C35-Ir1-Cl1	178.2(9)
P1-Ir1-Cl1	86.80(17)	P2-Ir1-Cl1	91.67(16)
C35A-Ir1-Cl1A	170.(3)	P1-Ir1-Cl1A	91.5(6)
P2-Ir1-Cl1A	90.3(6)	C35A-Ir1-Co1	89.(4)
C35-Ir1-Co1	83.2(8)	P1-Ir1-Co1	88.67(13)
P2-Ir1-Co1	86.58(13)	Cl1-Ir1-Co1	94.99(15)
Cl1A-Ir1-Co1	87.6(7)	C5-N1-C1	118.4(15)
C5-N1-Co1	127.5(11)	C1-N1-Co1	114.1(12)
C18-N2-C22	116.9(15)	C18-N2-Co1	117.4(13)
C22-N2-Co1	125.7(11)	C12-P1-C6	103.1(8)
C12-P1-C5	104.0(9)	C6-P1-C5	107.1(8)
C12-P1-Ir1	116.4(7)	C6-P1-Ir1	117.4(5)

C5-P1-Ir1	107.6(6)	C29-P2-C22	102.3(8)
C29-P2-C23	105.9(8)	C22-P2-C23	102.3(7)
C29-P2-Ir1	116.7(6)	C22-P2-Ir1	109.0(6)
C23-P2-Ir1	118.5(6)	Cl5-C36-Cl4	109.8(15)
Cl5-C36-H36A	109.7	Cl4-C36-H36A	109.7
Cl5-C36-H36B	109.7	Cl4-C36-H36B	109.7
H36A-C36-H36B	108.2	Cl7-C37-Cl6	114.7(14)
Cl7-C37-H37A	108.6	Cl6-C37-H37A	108.6
Cl7-C37-H37B	108.6	Cl6-C37-H37B	108.6
H37A-C37-H37B	107.6		

Table S15. Bond lengths (Å) for **3**.

C1-N1	1.34(2)	C1-C2	1.40(3)
C1-H1	0.95	C2-C3	1.34(3)
C2-H2	0.95	C3-C4	1.42(3)
C3-H3	0.95	C4-C5	1.38(2)
C4-H4	0.95	C5-N1	1.34(2)
C5-P1	1.843(18)	C6-C11	1.388(19)
C6-C7	1.404(19)	C6-P1	1.829(16)
C7-C8	1.382(19)	C7-H7	0.95
C8-C9	1.38(2)	C8-H8	0.95
C9-C10	1.35(2)	C9-H9	0.95
C10-C11	1.373(19)	C10-H10	0.95
C11-H11	0.95	C12-C17	1.41(3)
C12-C13	1.44(2)	C12-P1	1.782(19)
C13-C14	1.39(3)	C13-H13	0.95
C14-C15	1.38(3)	C14-H14	0.95
C15-C16	1.36(3)	C15-H15	0.95
C16-C17	1.37(3)	C16-H16	0.95
C17-H17	0.95	C18-N2	1.34(2)
C18-C19	1.40(3)	C18-H18	0.95
C19-C20	1.36(3)	C19-H19	0.95
C20-C21	1.38(3)	C20-H20	0.95
C21-C22	1.34(2)	C21-H21	0.95
C22-N2	1.37(2)	C22-P2	1.830(17)
C23-C28	1.37(2)	C23-C24	1.386(19)
C23-P2	1.833(17)	C24-C25	1.40(2)
C24-H24	0.95	C25-C26	1.38(2)
C25-H25	0.95	C26-C27	1.39(2)
C26-H26	0.95	C27-C28	1.394(19)
C27-H27	0.95	C28-H28	0.95
C29-C30	1.39(2)	C29-C34	1.387(19)
C29-P2	1.816(18)	C30-C31	1.39(2)
C30-H30	0.95	C31-C32	1.38(2)
C31-H31	0.95	C32-C33	1.38(2)

C32-H32	0.95	C33-C34	1.38(2)
C33-H33	0.95	C34-H34	0.95
C35-O1	1.15(3)	C35-Ir1	1.79(3)
C35A-O1A	1.17(4)	C35A-Ir1	1.79(4)
Cl1-Ir1	2.365(5)	Cl1A-Ir1	2.40(2)
Cl2-Co1	2.296(5)	Cl3-Co1	2.304(5)
Co1-N2	2.209(15)	Co1-N1	2.215(14)
Co1-Ir1	2.652(2)	Ir1-P1	2.316(4)
Ir1-P2	2.324(4)	C36-Cl5	1.77(2)
C36-Cl4	1.78(3)	C36-H36A	0.99
C36-H36B	0.99	C37-Cl7	1.73(3)
C37-Cl6	1.74(3)	C37-H37A	0.99
C37-H37B	0.99		

Table S16. Anisotropic atomic displacement parameters (Å^2) for **3**.

The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.043(8)	0.058(10)	0.049(9)	-0.003(7)	0.021(7)	0.003(7)
C2	0.061(10)	0.060(11)	0.059(11)	0.002(8)	0.031(8)	0.015(8)
C3	0.077(11)	0.063(12)	0.049(11)	-0.012(8)	0.030(9)	0.012(8)
C4	0.059(9)	0.056(10)	0.039(9)	-0.006(7)	0.014(8)	0.007(8)
C5	0.045(7)	0.053(9)	0.024(7)	-0.001(6)	0.007(6)	0.009(6)
C6	0.044(8)	0.046(8)	0.038(8)	-0.009(6)	0.011(6)	-0.004(6)
C7	0.054(9)	0.046(8)	0.048(9)	-0.010(7)	0.010(7)	-0.001(7)
C8	0.058(10)	0.052(9)	0.047(9)	-0.009(7)	0.010(7)	-0.008(7)
C9	0.055(10)	0.064(9)	0.041(9)	-0.009(7)	0.017(7)	-0.003(7)
C10	0.051(9)	0.061(8)	0.042(8)	-0.001(7)	0.019(7)	0.000(7)
C11	0.038(8)	0.050(8)	0.043(8)	0.000(6)	0.012(6)	-0.004(6)
C12	0.041(9)	0.042(8)	0.069(13)	0.005(7)	0.016(8)	0.001(6)
C13	0.050(9)	0.049(9)	0.049(10)	0.003(7)	0.010(8)	0.008(7)
C14	0.076(11)	0.053(10)	0.045(10)	0.005(7)	0.006(9)	0.001(9)
C15	0.097(12)	0.047(10)	0.041(10)	-0.002(7)	0.024(9)	-0.010(8)
C16	0.090(12)	0.057(11)	0.060(12)	0.002(8)	0.037(11)	-0.007(9)
C17	0.058(9)	0.050(9)	0.056(11)	-0.003(7)	0.029(9)	-0.004(7)
C18	0.053(9)	0.067(11)	0.035(8)	0.008(7)	0.012(6)	0.004(8)
C19	0.054(10)	0.070(12)	0.035(9)	0.001(7)	0.001(8)	-0.004(8)
C20	0.058(10)	0.062(11)	0.031(7)	-0.002(7)	0.012(7)	-0.005(7)
C21	0.060(10)	0.047(9)	0.036(8)	-0.004(6)	0.007(7)	0.003(8)
C22	0.043(7)	0.040(8)	0.035(7)	0.000(5)	0.013(6)	-0.008(6)
C23	0.065(9)	0.036(8)	0.044(8)	0.005(6)	0.022(7)	0.008(6)
C24	0.065(10)	0.043(9)	0.041(8)	0.002(7)	0.017(7)	0.005(7)
C25	0.071(10)	0.052(10)	0.047(10)	0.012(7)	0.021(8)	0.013(8)
C26	0.076(10)	0.049(10)	0.050(9)	0.006(7)	0.029(8)	0.006(8)
C27	0.075(11)	0.046(9)	0.044(9)	-0.001(7)	0.019(8)	-0.004(8)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C28	0.065(9)	0.044(9)	0.043(9)	0.003(7)	0.017(7)	0.002(7)
C29	0.053(9)	0.049(8)	0.034(8)	-0.006(6)	0.012(7)	0.008(7)
C30	0.073(12)	0.059(10)	0.057(12)	0.000(9)	0.031(10)	0.004(8)
C31	0.061(12)	0.082(11)	0.060(13)	-0.001(11)	0.023(10)	0.004(10)
C32	0.057(12)	0.088(12)	0.054(13)	-0.003(11)	0.014(10)	0.018(9)
C33	0.066(12)	0.070(11)	0.064(13)	-0.008(10)	0.021(10)	0.021(9)
C34	0.064(11)	0.051(8)	0.062(12)	-0.012(8)	0.021(9)	0.009(8)
C35	0.075(15)	0.026(9)	0.030(9)	-0.006(6)	0.025(8)	-0.002(8)
O1	0.063(10)	0.043(8)	0.025(8)	0.002(6)	0.020(7)	-0.004(7)
C35A	0.075(15)	0.026(9)	0.030(9)	-0.006(6)	0.025(8)	-0.002(8)
O1A	0.063(10)	0.043(8)	0.025(8)	0.002(6)	0.020(7)	-0.004(7)
Cl1	0.059(3)	0.037(3)	0.028(3)	0.000(2)	0.016(2)	0.000(2)
Cl1A	0.059(3)	0.037(3)	0.028(3)	0.000(2)	0.016(2)	0.000(2)
Cl2	0.064(3)	0.057(2)	0.039(2)	0.0147(18)	0.022(2)	0.011(2)
Cl3	0.051(2)	0.055(2)	0.0339(19)	0.0070(17)	0.0147(17)	-0.0049(19)
Co1	0.0362(11)	0.0437(11)	0.0263(10)	0.0041(9)	0.0106(8)	0.0022(10)
Ir1	0.0453(3)	0.0362(3)	0.0308(3)	-0.0019(4)	0.0127(2)	0.0003(4)
N1	0.040(6)	0.050(7)	0.036(7)	0.002(5)	0.015(5)	0.000(5)
N2	0.050(7)	0.049(8)	0.035(6)	0.000(6)	0.017(5)	-0.004(6)
P1	0.049(2)	0.034(2)	0.036(2)	-0.0024(16)	0.0148(19)	0.0024(17)
P2	0.050(2)	0.035(2)	0.029(2)	-0.0054(15)	0.0092(17)	0.0000(17)
C36	0.059(13)	0.100(18)	0.082(17)	-0.016(14)	0.033(12)	-0.018(12)
Cl4	0.077(4)	0.108(6)	0.084(5)	-0.015(4)	0.013(3)	0.014(4)
Cl5	0.069(4)	0.091(4)	0.092(5)	-0.027(4)	0.022(3)	-0.012(3)
C37	0.076(15)	0.078(15)	0.071(15)	-0.014(12)	0.029(12)	0.004(12)
Cl6	0.082(4)	0.080(4)	0.065(3)	-0.011(3)	0.026(3)	-0.002(3)
Cl7	0.088(4)	0.080(4)	0.080(4)	-0.001(3)	0.008(4)	-0.008(3)

Table S17. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for **3**.

	x/a	**y/b**	**z/c**	**U(eq)**
H1	0.3349	0.8221	0.5605	0.058
H2	0.3216	0.9342	0.6726	0.069
H3	0.4089	1.0281	0.7633	0.073
H4	0.5102	1.0163	0.7340	0.062
H7	0.5953	1.0960	0.6960	0.061
H8	0.6819	1.1459	0.8231	0.065
H9	0.7605	1.0221	0.8965	0.064
H10	0.7502	0.8497	0.8504	0.06
H11	0.6649	0.7965	0.7253	0.053
H13	0.4483	1.0446	0.4959	0.061
H14	0.4464	1.1818	0.3945	0.073
H15	0.5373	1.2181	0.3512	0.073
H16	0.6330	1.1295	0.4177	0.079

	x/a	y/b	z/c	U(eq)
H17	0.6403	0.9984	0.5229	0.062
H18	0.3466	0.6580	0.2882	0.063
H19	0.3478	0.5453	0.1706	0.067
H20	0.4343	0.4315	0.1862	0.062
H21	0.5227	0.4420	0.3206	0.06
H24	0.6172	0.4531	0.6529	0.06
H25	0.5927	0.3174	0.7390	0.067
H26	0.4913	0.2353	0.6898	0.068
H27	0.4118	0.2968	0.5580	0.067
H28	0.4377	0.4305	0.4719	0.061
H30	0.6463	0.6588	0.4263	0.073
H31	0.7306	0.6032	0.3753	0.08
H32	0.7606	0.4265	0.3845	0.08
H33	0.6994	0.3022	0.4334	0.08
H34	0.6151	0.3581	0.4844	0.071
H36A	0.2640	0.4043	0.2078	0.093
H36B	0.3122	0.3414	0.1666	0.093
H37A	0.8211	0.6883	0.6698	0.088
H37B	0.7889	0.6241	0.5779	0.088

Crystal Structure of 4

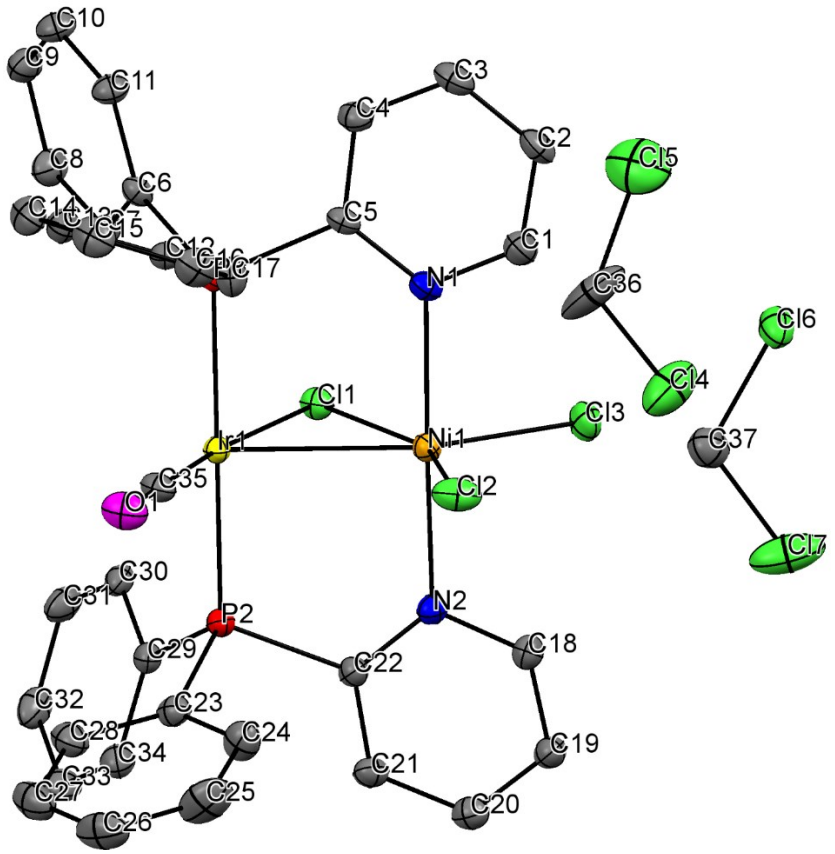


Figure S17. Molecular structure of **4** shown with 50% probability ellipsoids.

A red needle-like specimen of $C_{37}H_{32}Cl_7IrN_2NiOP_2$, approximate dimensions 0.105 mm x 0.137 mm x 0.289 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured on a Bruker APEX II CCD Bruker APEX DUO system equipped with a fine-focus tube (MoKα , λ = 0.71073 Å) and a TRIUMPH curved-crystal monochromator.

The frames were integrated with the Bruker SAINT software package using a SAINT V8.40A (Bruker AXS, 2013) algorithm. The integration of the data using a monoclinic unit cell yielded a total of 95672 reflections to a maximum θ angle of 29.57° (0.72 Å resolution), of which 11264 were independent (average redundancy 8.494, completeness = 99.9%, R_{int} = 6.42%, R_{sig} = 3.55%) and 9735 (86.43%) were greater than $2\sigma(F^2)$. The final cell constants of a = 9.717(4) Å, b = 16.846(6) Å, c = 24.683(9) Å, β = 99.673(6)°, volume = 3983.(2) $Å^3$, are based upon the refinement of the XYZ-centroids of 9679 reflections above 20 σ(I) with 4.824° < 2θ < 60.58°. Data were corrected for absorption effects using the multi-scan method (SADABS). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.0590 and 0.0998.

The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P 1 21/n 1, with Z = 4 for the formula unit, $C_{37}H_{32}Cl_7IrN_2NiOP_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 481 variables converged at R1 = 3.88%, for the observed data and wR2 = 9.03% for all data. The goodness-of-fit was 1.121. The largest peak in the final difference electron density synthesis was 2.366 $e^-/Å^3$ and the largest hole was -1.278 $e^-/Å^3$ with an RMS deviation of 0.159 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.804 g/cm^3 and F(000), 2120 e^-.

Table S18. Sample and crystal data for **4**.

Identification code	Val	
Chemical formula	$C_{37}H_{32}Cl_7IrN_2NiOP_2$	
Formula weight	1081.64 g/mol	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal size	0.105 x 0.137 x 0.289 mm	
Crystal habit	red needle	
Crystal system	monoclinic	
Space group	P 1 21/n 1	
Unit cell dimensions	a = 9.717(4) Å	α = 90°
	b = 16.846(6) Å	β = 99.673(6)°
	c = 24.683(9) Å	γ = 90°
Volume	3983.(2) $Å^3$	
Z	4	
Density (calculated)	1.804 g/cm^3	
Absorption coefficient	4.394 mm^{-1}	
F(000)	2120	

Table S19. Data collection and structure refinement for **4**.

Diffractometer	Bruker APEX II CCD Bruker APEX DUO	
Radiation source	fine-focus tube (MoKα , λ = 0.71073 Å)	
Theta range for data collection	2.15 to 29.57°	
Index ranges	-13<=h<=13, -23<=k<=23, -34<=l<=34	
Reflections collected	95672	
Independent reflections	11264 [R(int) = 0.0642]	
Coverage of independent reflections	99.9%	
Absorption correction	multi-scan	
Max. and min. transmission	0.0998 and 0.0590	
Structure solution technique	direct methods	
Structure solution program	SHELXTL XT 2014/5 (Bruker AXS, 2014)	
Refinement method	Full-matrix least-squares on F^2	
Refinement program	SHELXL-2018/3 (Sheldrick, 2018)	
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$	
Data / restraints / parameters	11264 / 18 / 481	
Goodness-of-fit on F^2	1.121	
Δ/σ_{max}	0.002	
Final R indices	9735 data; I>2σ(I)	R1 = 0.0388, wR2 = 0.0851
	all data	R1 = 0.0500, wR2 = 0.0903
Weighting scheme	$w=1/[\sigma^2(F_o^2)+36.4461P]$ where $P=(F_o^2+2F_c^2)/3$	
Largest diff. peak and hole	2.366 and -1.278 $eÅ^{-3}$	
R.M.S. deviation from mean	0.159 $eÅ^{-3}$	

Table S20. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x/a	y/b	z/c	U(eq)
C1	0.5257(6)	0.4939(3)	0.2515(2)	0.0219(11)
C2	0.4998(6)	0.4137(3)	0.2400(2)	0.0228(11)
C3	0.5900(6)	0.3578(3)	0.2668(2)	0.0225(10)
C4	0.7004(6)	0.3836(3)	0.3062(2)	0.0197(10)
C5	0.7177(5)	0.4649(3)	0.3172(2)	0.0146(9)
C6	0.0113(5)	0.4518(3)	0.3712(2)	0.0158(9)
C7	0.1209(5)	0.5000(3)	0.3613(2)	0.0187(10)
C8	0.2496(6)	0.4676(3)	0.3564(2)	0.0229(11)
C9	0.2687(6)	0.3852(3)	0.3610(2)	0.0230(11)
C10	0.1606(6)	0.3370(3)	0.3704(2)	0.0216(11)
C11	0.0332(5)	0.3695(3)	0.3764(2)	0.0193(10)
C12	0.7780(5)	0.4485(3)	0.4314(2)	0.0146(9)
C13	0.8665(6)	0.4147(3)	0.4760(2)	0.0198(10)
C14	0.8111(6)	0.3807(3)	0.5187(2)	0.0243(11)
C15	0.6674(6)	0.3808(3)	0.5185(2)	0.0264(12)
C16	0.5796(6)	0.4146(4)	0.4746(2)	0.0257(12)
C17	0.6345(6)	0.4486(3)	0.4312(2)	0.0208(11)
C18	0.5360(5)	0.8118(3)	0.2726(2)	0.0186(10)
C19	0.5235(6)	0.8935(3)	0.2678(2)	0.0197(10)
C20	0.6250(6)	0.9410(3)	0.2978(2)	0.0214(11)
C21	0.7324(6)	0.9049(3)	0.3331(2)	0.0194(10)
C22	0.7370(5)	0.8223(3)	0.3371(2)	0.0164(9)
C23	0.7966(6)	0.8088(3)	0.4528(2)	0.0185(10)
C24	0.6531(6)	0.8161(4)	0.4517(2)	0.0252(12)
C25	0.6029(8)	0.8370(4)	0.4989(3)	0.0386(16)
C26	0.6948(8)	0.8505(4)	0.5472(2)	0.0350(15)
C27	0.8370(8)	0.8424(4)	0.5491(2)	0.0311(13)
C28	0.8883(7)	0.8206(3)	0.5017(2)	0.0246(11)
C29	0.0282(5)	0.8206(3)	0.3929(2)	0.0158(9)
C30	0.1348(5)	0.7796(3)	0.3733(2)	0.0178(10)
C31	0.2652(6)	0.8143(3)	0.3739(2)	0.0235(11)
C32	0.2893(6)	0.8914(3)	0.3947(3)	0.0259(12)
C33	0.1854(6)	0.9326(3)	0.4141(2)	0.0252(12)
C34	0.0559(6)	0.8980(3)	0.4137(2)	0.0219(11)
C35	0.7909(5)	0.6288(3)	0.4496(2)	0.0181(9)
Cl1	0.89786(13)	0.64550(7)	0.29172(5)	0.0176(2)
Cl2	0.45083(15)	0.64323(8)	0.34113(6)	0.0256(3)
Cl3	0.57209(15)	0.66191(8)	0.20164(5)	0.0243(3)
Ir1	0.85265(2)	0.63583(2)	0.38346(2)	0.01277(5)
N1	0.6332(4)	0.5203(3)	0.28891(18)	0.0172(8)
N2	0.6421(4)	0.7750(3)	0.30523(18)	0.0157(8)
Ni1	0.64162(7)	0.64762(4)	0.29731(3)	0.01510(13)

	x/a	y/b	z/c	U(eq)
O1	0.7484(4)	0.6244(2)	0.48994(16)	0.0261(9)
P1	0.84456(14)	0.49865(7)	0.37607(5)	0.0139(2)
P2	0.85938(14)	0.77272(7)	0.39148(5)	0.0144(2)
C36	0.8108(13)	0.6286(6)	0.1084(4)	0.051(3)
Cl4	0.7730(6)	0.7183(3)	0.0715(2)	0.0470(10)
Cl5	0.8149(8)	0.5473(2)	0.06421(18)	0.0582(13)
C36A	0.768(4)	0.6326(12)	0.1057(11)	0.051(3)
Cl4A	0.8150(14)	0.7256(9)	0.0807(7)	0.0470(10)
Cl5A	0.7487(19)	0.5539(8)	0.0590(6)	0.0582(13)
C37	0.2077(15)	0.6262(7)	0.2315(5)	0.029(3)
Cl6	0.1781(11)	0.5477(5)	0.1823(2)	0.0278(10)
Cl7	0.1410(6)	0.7165(2)	0.2031(2)	0.0525(12)
C37A	0.203(2)	0.6468(10)	0.2167(9)	0.029(3)
Cl6A	0.176(2)	0.5465(9)	0.1959(4)	0.0278(10)
Cl7A	0.0801(9)	0.7090(4)	0.1782(4)	0.0525(12)

Table S21. Bond lengths (Å) for **4**.

C1-N1	1.348(7)	C1-C2	1.394(8)
C1-H1	0.95	C2-C3	1.378(8)
C2-H2	0.95	C3-C4	1.390(7)
C3-H3	0.95	C4-C5	1.402(7)
C4-H4	0.95	C5-N1	1.355(7)
C5-P1	1.831(5)	C6-C7	1.392(7)
C6-C11	1.407(7)	C6-P1	1.824(5)
C7-C8	1.389(7)	C7-H7	0.95
C8-C9	1.402(8)	C8-H8	0.95
C9-C10	1.378(8)	C9-H9	0.95
C10-C11	1.384(7)	C10-H10	0.95
C11-H11	0.95	C12-C17	1.394(7)
C12-C13	1.399(7)	C12-P1	1.815(5)
C13-C14	1.385(7)	C13-H13	0.95
C14-C15	1.396(8)	C14-H14	0.95
C15-C16	1.385(8)	C15-H15	0.95
C16-C17	1.397(8)	C16-H16	0.95
C17-H17	0.95	C18-N2	1.347(6)
C18-C19	1.385(7)	C18-H18	0.95
C19-C20	1.385(8)	C19-H19	0.95
C20-C21	1.382(8)	C20-H20	0.95
C21-C22	1.395(7)	C21-H21	0.95
C22-N2	1.364(7)	C22-P2	1.837(5)
C23-C28	1.389(8)	C23-C24	1.395(8)
C23-P2	1.829(5)	C24-C25	1.382(8)
C24-H24	0.95	C25-C26	1.383(10)
C25-H25	0.95	C26-C27	1.381(10)

C26-H26	0.95	C27-C28	1.395(8)
C27-H27	0.95	C28-H28	0.95
C29-C30	1.397(7)	C29-C34	1.409(7)
C29-P2	1.824(5)	C30-C31	1.393(7)
C30-H30	0.95	C31-C32	1.400(8)
C31-H31	0.95	C32-C33	1.376(8)
C32-H32	0.95	C33-C34	1.385(8)
C33-H33	0.95	C34-H34	0.95
C35-O1	1.143(6)	C35-Ir1	1.834(5)
Cl1-Ir1	2.3837(14)	Cl1-Ni1	2.5170(16)
Cl2-Ni1	2.2990(15)	Cl3-Ni1	2.3569(16)
Ir1-P2	2.3146(15)	Ir1-P1	2.3184(15)
Ir1-Ni1	2.7019(10)	N1-Ni1	2.156(4)
N2-Ni1	2.155(4)	C36-Cl5	1.756(10)
C36-Cl4	1.771(9)	C36-H36A	0.99
C36-H36B	0.99	C36A-Cl5A	1.747(16)
C36A-Cl4A	1.772(16)	C36A-H36C	0.99
C36A-H36D	0.99	C37-Cl7	1.753(10)
C37-Cl6	1.785(10)	C37-H37A	0.99
C37-H37B	0.99	C37A-Cl7A	1.747(15)
C37A-Cl6A	1.772(14)	C37A-H37C	0.99
C37A-H37D	0.99		

Table S22. Bond angles (°) for **4**.

N1-C1-C2	123.4(5)	N1-C1-H1	118.3
C2-C1-H1	118.3	C3-C2-C1	119.2(5)
C3-C2-H2	120.4	C1-C2-H2	120.4
C2-C3-C4	118.4(5)	C2-C3-H3	120.8
C4-C3-H3	120.8	C3-C4-C5	119.6(5)
C3-C4-H4	120.2	C5-C4-H4	120.2
N1-C5-C4	122.0(5)	N1-C5-P1	117.7(4)
C4-C5-P1	120.0(4)	C7-C6-C11	118.9(5)
C7-C6-P1	118.3(4)	C11-C6-P1	122.9(4)
C8-C7-C6	120.8(5)	C8-C7-H7	119.6
C6-C7-H7	119.6	C7-C8-C9	119.4(5)
C7-C8-H8	120.3	C9-C8-H8	120.3
C10-C9-C8	120.2(5)	C10-C9-H9	119.9
C8-C9-H9	119.9	C9-C10-C11	120.4(5)
C9-C10-H10	119.8	C11-C10-H10	119.8
C10-C11-C6	120.3(5)	C10-C11-H11	119.9
C6-C11-H11	119.9	C17-C12-C13	119.1(5)
C17-C12-P1	118.7(4)	C13-C12-P1	122.1(4)
C14-C13-C12	120.1(5)	C14-C13-H13	120.0
C12-C13-H13	120.0	C13-C14-C15	120.9(5)
C13-C14-H14	119.5	C15-C14-H14	119.5

C16-C15-C14	119.1(5)	C16-C15-H15	120.4
C14-C15-H15	120.4	C15-C16-C17	120.4(5)
C15-C16-H16	119.8	C17-C16-H16	119.8
C12-C17-C16	120.5(5)	C12-C17-H17	119.8
C16-C17-H17	119.8	N2-C18-C19	123.7(5)
N2-C18-H18	118.1	C19-C18-H18	118.1
C18-C19-C20	119.0(5)	C18-C19-H19	120.5
C20-C19-H19	120.5	C21-C20-C19	118.5(5)
C21-C20-H20	120.8	C19-C20-H20	120.8
C20-C21-C22	119.7(5)	C20-C21-H21	120.1
C22-C21-H21	120.1	N2-C22-C21	122.0(5)
N2-C22-P2	116.6(4)	C21-C22-P2	121.0(4)
C28-C23-C24	119.9(5)	C28-C23-P2	120.8(4)
C24-C23-P2	118.9(4)	C25-C24-C23	119.9(6)
C25-C24-H24	120.1	C23-C24-H24	120.1
C24-C25-C26	120.0(6)	C24-C25-H25	120.0
C26-C25-H25	120.0	C27-C26-C25	120.7(6)
C27-C26-H26	119.6	C25-C26-H26	119.6
C26-C27-C28	119.5(6)	C26-C27-H27	120.2
C28-C27-H27	120.2	C23-C28-C27	119.9(6)
C23-C28-H28	120.0	C27-C28-H28	120.0
C30-C29-C34	118.4(5)	C30-C29-P2	119.4(4)
C34-C29-P2	122.1(4)	C31-C30-C29	121.0(5)
C31-C30-H30	119.5	C29-C30-H30	119.5
C30-C31-C32	119.3(5)	C30-C31-H31	120.4
C32-C31-H31	120.4	C33-C32-C31	120.5(5)
C33-C32-H32	119.8	C31-C32-H32	119.8
C32-C33-C34	120.3(5)	C32-C33-H33	119.9
C34-C33-H33	119.9	C33-C34-C29	120.6(5)
C33-C34-H34	119.7	C29-C34-H34	119.7
O1-C35-Ir1	177.9(5)	Ir1-Cl1-Ni1	66.85(3)
C35-Ir1-P2	89.84(16)	C35-Ir1-P1	89.63(16)
P2-Ir1-P1	179.45(5)	C35-Ir1-Cl1	171.67(17)
P2-Ir1-Cl1	90.35(4)	P1-Ir1-Cl1	90.15(4)
C35-Ir1-Ni1	112.74(17)	P2-Ir1-Ni1	90.05(4)
P1-Ir1-Ni1	90.01(3)	Cl1-Ir1-Ni1	58.93(4)
C1-N1-C5	117.3(4)	C1-N1-Ni1	113.9(4)
C5-N1-Ni1	128.7(3)	C18-N2-C22	116.8(4)
C18-N2-Ni1	114.5(3)	C22-N2-Ni1	128.7(3)
N2-Ni1-N1	177.99(16)	N2-Ni1-Cl2	88.80(12)
N1-Ni1-Cl2	89.59(12)	N2-Ni1-Cl3	89.14(12)
N1-Ni1-Cl3	90.30(13)	Cl2-Ni1-Cl3	110.89(6)
N2-Ni1-Cl1	91.83(12)	N1-Ni1-Cl1	90.13(12)
Cl2-Ni1-Cl1	155.32(6)	Cl3-Ni1-Cl1	93.79(5)
N2-Ni1-Ir1	90.69(12)	N1-Ni1-Ir1	90.80(12)

Cl2-Ni1-Ir1	101.12(5)	Cl3-Ni1-Ir1	147.98(5)
Cl1-Ni1-Ir1	54.21(3)	C12-P1-C6	106.3(2)
C12-P1-C5	100.1(2)	C6-P1-C5	107.5(2)
C12-P1-Ir1	114.61(16)	C6-P1-Ir1	114.67(17)
C5-P1-Ir1	112.40(17)	C29-P2-C23	105.2(2)
C29-P2-C22	106.4(2)	C23-P2-C22	100.8(2)
C29-P2-Ir1	117.07(17)	C23-P2-Ir1	113.18(17)
C22-P2-Ir1	112.66(17)	Cl5-C36-Cl4	111.7(6)
Cl5-C36-H36A	109.3	Cl4-C36-H36A	109.3
Cl5-C36-H36B	109.3	Cl4-C36-H36B	109.3
H36A-C36-H36B	107.9	Cl5A-C36A-Cl4A	116.5(15)
Cl5A-C36A-H36C	108.2	Cl4A-C36A-H36C	108.2
Cl5A-C36A-H36D	108.2	Cl4A-C36A-H36D	108.2
H36C-C36A-H36D	107.3	Cl7-C37-Cl6	111.4(7)
Cl7-C37-H37A	109.3	Cl6-C37-H37A	109.3
Cl7-C37-H37B	109.3	Cl6-C37-H37B	109.3
H37A-C37-H37B	108.0	Cl7A-C37A-Cl6A	111.0(12)
Cl7A-C37A-H37C	109.4	Cl6A-C37A-H37C	109.4
Cl7A-C37A-H37D	109.4	Cl6A-C37A-H37D	109.4
H37C-C37A-H37D	108.0		

Table S23. Anisotropic atomic displacement parameters (Å^2) for **4**.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.021(3)	0.022(3)	0.023(3)	-0.003(2)	0.002(2)	0.000(2)
C2	0.021(3)	0.024(3)	0.022(3)	-0.008(2)	0.001(2)	-0.006(2)
C3	0.029(3)	0.018(2)	0.022(2)	-0.005(2)	0.007(2)	-0.007(2)
C4	0.026(3)	0.015(2)	0.018(2)	0.0009(18)	0.005(2)	-0.0010(19)
C5	0.017(2)	0.013(2)	0.015(2)	-0.0027(18)	0.0059(18)	-0.0034(18)
C6	0.017(2)	0.017(2)	0.014(2)	-0.0027(18)	0.0043(18)	-0.0016(18)
C7	0.017(2)	0.017(2)	0.021(2)	0.0019(19)	-0.0012(19)	0.0014(19)
C8	0.015(2)	0.022(3)	0.032(3)	0.000(2)	0.003(2)	-0.002(2)
C9	0.019(2)	0.021(3)	0.029(3)	0.000(2)	0.002(2)	0.003(2)
C10	0.025(3)	0.015(2)	0.026(3)	0.003(2)	0.007(2)	0.002(2)
C11	0.021(2)	0.015(2)	0.023(2)	0.002(2)	0.0063(19)	0.000(2)
C12	0.016(2)	0.013(2)	0.016(2)	-0.0002(17)	0.0032(18)	-0.0002(17)
C13	0.020(2)	0.021(2)	0.018(2)	0.001(2)	0.0027(19)	0.001(2)
C14	0.031(3)	0.023(3)	0.018(2)	0.005(2)	0.004(2)	-0.002(2)
C15	0.035(3)	0.025(3)	0.021(3)	0.003(2)	0.011(2)	-0.006(2)
C16	0.022(3)	0.029(3)	0.028(3)	-0.003(2)	0.010(2)	-0.002(2)
C17	0.018(2)	0.026(3)	0.018(2)	0.001(2)	0.0009(19)	-0.001(2)
C18	0.017(2)	0.020(2)	0.019(2)	0.001(2)	0.0017(19)	0.0011(19)
C19	0.022(3)	0.019(2)	0.018(2)	0.0008(19)	0.003(2)	0.004(2)
C20	0.026(3)	0.019(2)	0.020(2)	0.001(2)	0.007(2)	0.002(2)
C21	0.020(2)	0.017(2)	0.022(3)	-0.002(2)	0.005(2)	0.002(2)

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C22	0.019(2)	0.017(2)	0.014(2)	0.0001(18)	0.0033(18)	0.0021(19)
C23	0.025(3)	0.016(2)	0.015(2)	0.0017(19)	0.005(2)	0.003(2)
C24	0.027(3)	0.032(3)	0.017(2)	0.001(2)	0.008(2)	0.006(2)
C25	0.045(4)	0.044(4)	0.033(3)	0.006(3)	0.024(3)	0.019(3)
C26	0.061(4)	0.027(3)	0.021(3)	0.000(2)	0.020(3)	0.006(3)
C27	0.049(4)	0.026(3)	0.018(3)	-0.002(2)	0.005(3)	-0.004(3)
C28	0.033(3)	0.019(3)	0.021(3)	-0.001(2)	0.003(2)	-0.003(2)
C29	0.016(2)	0.016(2)	0.015(2)	0.0003(18)	-0.0004(18)	0.0007(18)
C30	0.017(2)	0.016(2)	0.020(2)	0.0033(19)	0.0001(19)	0.0018(19)
C31	0.016(2)	0.022(3)	0.033(3)	0.003(2)	0.004(2)	0.003(2)
C32	0.016(2)	0.023(3)	0.037(3)	0.007(2)	-0.001(2)	-0.004(2)
C33	0.028(3)	0.016(2)	0.030(3)	0.000(2)	0.001(2)	-0.004(2)
C34	0.023(3)	0.019(2)	0.022(3)	0.001(2)	0.001(2)	-0.001(2)
C35	0.023(2)	0.014(2)	0.018(2)	-0.0020(19)	0.0053(19)	-0.002(2)
Cl1	0.0208(5)	0.0170(5)	0.0158(5)	0.0006(4)	0.0054(4)	-0.0006(4)
Cl2	0.0293(6)	0.0188(6)	0.0329(7)	-0.0035(5)	0.0170(5)	-0.0036(5)
Cl3	0.0281(7)	0.0295(7)	0.0143(5)	-0.0004(5)	0.0010(5)	0.0030(5)
Ir1	0.01376(8)	0.01195(8)	0.01257(8)	-0.00006(7)	0.00217(6)	0.00002(7)
N1	0.016(2)	0.017(2)	0.019(2)	-0.0033(17)	0.0039(16)	-0.0019(16)
N2	0.0140(19)	0.016(2)	0.018(2)	0.0002(16)	0.0033(16)	0.0004(16)
Ni1	0.0165(3)	0.0147(3)	0.0140(3)	-0.0005(2)	0.0022(2)	-0.0002(2)
O1	0.033(2)	0.025(2)	0.0238(19)	-0.0007(16)	0.0148(17)	-0.0027(17)
P1	0.0148(6)	0.0137(5)	0.0132(6)	0.0001(4)	0.0020(5)	-0.0010(5)
P2	0.0151(6)	0.0139(5)	0.0141(6)	-0.0002(5)	0.0022(5)	0.0008(5)
C36	0.059(9)	0.049(5)	0.054(5)	0.030(4)	0.037(6)	0.038(5)
Cl4	0.035(2)	0.0435(15)	0.064(2)	0.0206(15)	0.013(2)	0.0090(18)
Cl5	0.087(4)	0.0464(14)	0.0465(15)	0.0101(11)	0.026(2)	-0.007(2)
C36A	0.059(9)	0.049(5)	0.054(5)	0.030(4)	0.037(6)	0.038(5)
Cl4A	0.035(2)	0.0435(15)	0.064(2)	0.0206(15)	0.013(2)	0.0090(18)
Cl5A	0.087(4)	0.0464(14)	0.0465(15)	0.0101(11)	0.026(2)	-0.007(2)
C37	0.027(3)	0.030(7)	0.031(7)	-0.003(5)	0.005(5)	-0.001(5)
Cl6	0.0312(9)	0.0259(8)	0.024(3)	0.004(2)	-0.002(3)	-0.0046(6)
Cl7	0.067(3)	0.0271(12)	0.076(3)	0.0106(19)	0.047(2)	0.0090(18)
C37A	0.027(3)	0.030(7)	0.031(7)	-0.003(5)	0.005(5)	-0.001(5)
Cl6A	0.0312(9)	0.0259(8)	0.024(3)	0.004(2)	-0.002(3)	-0.0046(6)
Cl7A	0.067(3)	0.0271(12)	0.076(3)	0.0106(19)	0.047(2)	0.0090(18)

Table S24. Hydrogen atomic coordinates and isotropic atomic displacement parameters (Å^2) for **4**.

	x/a	y/b	z/c	U(eq)
H1	0.4643	0.5320	0.2319	0.026
H2	0.4210	0.3979	0.2141	0.027
H3	0.5772	0.3029	0.2585	0.027
H4	0.7636	0.3462	0.3255	0.024
H7	1.1074	0.5558	0.3579	0.022

	x/a	y/b	z/c	U(eq)
H8	1.3240	0.5009	0.3499	0.028
H9	1.3564	0.3626	0.3577	0.028
H10	1.1736	0.2811	0.3728	0.026
H11	0.9602	0.3360	0.3841	0.023
H13	0.9647	0.4151	0.4770	0.024
H14	0.8718	0.3571	0.5485	0.029
H15	0.6303	0.3579	0.5482	0.032
H16	0.4816	0.4146	0.4739	0.031
H17	0.5735	0.4721	0.4014	0.025
H18	0.4656	0.7799	0.2518	0.022
H19	0.4465	0.9166	0.2443	0.024
H20	0.6210	0.9972	0.2942	0.026
H21	0.8027	0.9362	0.3545	0.023
H24	0.5900	0.8067	0.4185	0.03
H25	0.5052	0.8420	0.4982	0.046
H26	0.6598	0.8656	0.5794	0.042
H27	0.8994	0.8517	0.5824	0.037
H28	0.9858	0.8138	0.5029	0.029
H30	1.1182	0.7273	0.3594	0.021
H31	1.3369	0.7861	0.3604	0.028
H32	1.3780	0.9154	0.3953	0.031
H33	1.2026	0.9849	0.4280	0.03
H34	0.9850	0.9267	0.4275	0.026
H36A	0.9023	0.6334	0.1328	0.061
H36B	0.7389	0.6192	0.1318	0.061
H36C	0.8405	0.6176	0.1374	0.061
H36D	0.6793	0.6392	0.1197	0.061
H37A	0.1626	0.6130	0.2634	0.035
H37B	0.3092	0.6318	0.2447	0.035
H37C	0.1966	0.6517	0.2561	0.035
H37D	0.2982	0.6634	0.2119	0.035