Supporting Information for

Cooperative Bimetallic Reactivity: Hydrogen Activation in Two–Electron Mixed-Valence Compounds

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X-ray crystal structure solution of $(tfepma)_3Ir_2^{0,II}H_2Cl_2 \bullet 3CH_3CN$ (**B**). S2-S16

Atom numbering scheme for compounds **1-10** S17-S26

Table S1. Crystal data, structure solution and refinement for $(tfepma)_3Ir_2^{0,II}H_2Cl_2 \bullet 3CH_3CN$.

identification code	new
empirical formula	$C_{33}H_{42}Cl_2F_{36}Ir_2N_6O_{12}P_6$
formula weight	2039.85
T (K)	193(2)
λ (Å)	0.71073
crystal system	Monoclinic
space group	P2(1)/c
a (Å)	12.3635(15)
b (Å)	23.491(3)
c (Å)	23.867(3)
α (deg)	90
β (deg)	99.908(2)
γ (deg)	90
V (Å^3)	6828.3(14)
Z	4
ρ_{calcd} (Mg mm^{-3})	1.984
crystal size (mm^3)	0.40 × 0.29 × 0.28
abs coeff (mm^{-1})	4.264
F(000)	3920
θ range for data collection	2.19 to 23.31°
limiting indices	$-13 \leq h \leq 13$, $-26 \leq k \leq 22$, $-23 \leq \ell \leq 26$
no. of reflns collcd	25493
no. of ind reflns (R_{int})	9759 (0.0532)
completeness to $\theta = 23.25°$	99.8 %
absorption corr	SADABS
refinement method	Full-matrix least-squares on F^2
data / restraints / parameters	9759/ 12 / 797
$R1$,[a] $wR2$[b] [I > 2σ]	0.0919, 0.2049
$R1$,[a] $wR2$[b] (all data)	0.1008, 0.2091
GOF[c] on F^2	1.284
extinction coefficient	
largest diff. peak and hole	4.780 and –2.610 eÅ^{-3}

[a] $R1 = \Sigma||F_o - |F_c||/\Sigma|F_o|$. [b] $wR2 = (\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma(w(F_o^2)^2))^{1/2}$. [c] $GOF = (\Sigma\, w(F_o^2 - F_c^2)^2/(n - p))^{1/2}$ where n is the number of data and p is the number of parameters refined.

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $(tfepma)_3Ir_2^{0,II}H_2Cl_2 \bullet 3CH_3CN$.

Atom	x	y	z	U_{eq}[a]
Ir(1)	3229(1)	4069(1)	2497(1)	27(1)
Ir(2)	3688(1)	5211(1)	2465(1)	27(1)
Cl(1)	4011(4)	5252(2)	3501(2)	43(1)
Cl(2)	4513(4)	6168(2)	2489(2)	44(1)
P(1)	3692(3)	5215(2)	1563(2)	30(1)
P(2)	2599(3)	4155(2)	1543(2)	30(1)
P(3)	1924(3)	5458(2)	2485(2)	33(1)
P(4)	1608(3)	4280(2)	2757(2)	34(1)
P(5)	3503(4)	3141(2)	2722(2)	34(1)
P(6)	4947(3)	3795(2)	2406(2)	28(1)
O(1)	4807(9)	5345(5)	1347(5)	41(3)
O(2)	2961(10)	5666(5)	1168(5)	40(3)
O(3)	2627(10)	3649(5)	1097(6)	48(3)
O(4)	1329(9)	4329(5)	1419(4)	34(3)
O(5)	1615(10)	5909(6)	2944(6)	50(3)
O(6)	1260(10)	5722(5)	1902(6)	43(3)
O(7)	1522(10)	4132(5)	3406(6)	45(3)
O(8)	560(11)	3921(5)	2465(6)	50(3)
O(9)	3482(11)	2876(5)	3331(5)	46(3)
O(10)	2899(9)	2631(4)	2373(5)	37(3)
O(11)	6091(9)	4029(5)	2737(6)	42(3)
O(12)	5222(10)	3758(6)	1788(6)	50(3)
N(1)	3253(11)	4625(6)	1205(6)	34(3)
N(2)	1114(11)	4929(6)	2670(6)	34(3)
N(3)	4846(12)	3131(6)	2661(7)	43(4)
C(1)	3353(17)	4593(9)	584(8)	50(5)
C(2)	–8(17)	5031(8)	2783(9)	51(5)
C(3)	5650(14)	2690(7)	2774(9)	43(5)

C(4)	5897(12)	5281(7)	1659(8)	35(4)
C(5)	6653(15)	5588(10)	1342(11)	58(6)
C(6)	3256(19)	6239(8)	1130(9)	54(5)
C(7)	3120(30)	6394(12)	531(13)	98(10)
C(8)	2080(20)	3122(8)	1123(9)	66(7)
C(9)	1660(30)	2930(11)	562(11)	77(8)
C(10)	806(15)	4567(9)	887(9)	48(5)
C(11)	–401(18)	4518(11)	858(10)	61(6)
C(12)	2280(18)	6395(8)	3122(11)	60(6)
C(13)	1900(30)	6621(13)	3625(16)	93(9)
C(14)	228(16)	6006(9)	1846(11)	61(6)
C(15)	130(20)	6384(14)	1354(15)	87(9)
C(16)	1971(17)	4444(10)	3881(8)	53(5)
C(17)	1380(30)	4335(16)	4343(11)	83(8)
C(18)	390(20)	3355(13)	2663(13)	92(9)
C(19)	–610(30)	3102(14)	2359(16)	310(40)
C(20)	4040(20)	3090(10)	3845(9)	65(6)
C(22)	3021(16)	2039(8)	2495(8)	46(5)
C(23)	2019(19)	1742(8)	2222(11)	58(6)
C(24)	6180(15)	4259(9)	3282(8)	47(5)
C(25)	7250(20)	4594(13)	3402(10)	72(7)
C(26)	6020(20)	3411(10)	1611(10)	67(6)
C(27)	6220(20)	3547(11)	1063(11)	70(7)
F(1)	7668(10)	5526(7)	1611(7)	85(4)
F(2)	6438(11)	6134(5)	1298(7)	80(4)
F(3)	6610(12)	5388(7)	824(6)	86(5)
F(4)	3780(20)	6086(8)	259(7)	132(8)
F(5)	2135(19)	6326(8)	232(7)	128(8)
F(6)	3400(18)	6928(7)	448(8)	124(7)
F(7)	979(19)	3258(8)	253(9)	143(9)
F(8)	2460(20)	2892(11)	252(9)	167(10)

F(9)	1230(20)	2411(7)	551(8)	148(9)
F(10)	–715(11)	3966(7)	874(7)	90(5)
F(11)	–936(12)	4741(7)	390(7)	102(5)
F(12)	–739(11)	4754(8)	1295(7)	96(5)
F(13)	2459(17)	7099(10)	3784(12)	184(13)
F(14)	1990(30)	6297(13)	4040(9)	173(11)
F(15)	848(14)	6792(7)	3506(9)	111(6)
F(16)	–881(15)	6640(9)	1273(9)	139(8)
F(17)	849(16)	6781(8)	1387(10)	132(8)
F(18)	183(17)	6096(11)	871(9)	138(8)
F(19)	1460(20)	3795(12)	4490(8)	150(9)
F(20)	1740(19)	4584(11)	4810(7)	143(9)
F(21)	318(16)	4391(13)	4213(8)	155(10)
F(22)	–818(16)	2612(9)	2576(8)	124(6)
F(23)	–1430(30)	3444(17)	2366(15)	231(14)
F(24)	–530(30)	3103(16)	1815(16)	235(15)
F(28)	1187(11)	1895(7)	2453(7)	95(5)
F(29)	2145(12)	1188(5)	2308(7)	90(5)
F(30)	1778(12)	1835(6)	1670(7)	85(4)
F(31)	7382(13)	4827(8)	3918(7)	110(6)
F(32)	8097(11)	4246(8)	3377(8)	107(6)
F(33)	7275(12)	5004(7)	3022(7)	98(5)
F(34)	6401(18)	4080(7)	969(8)	120(7)
F(35)	6960(15)	3263(7)	875(7)	106(6)
F(36)	5252(17)	3456(9)	668(8)	118(6)
C(1S)	3830(30)	1284(13)	969(13)	95(9)
C(2S)	4210(20)	1824(13)	1181(12)	79(7)
C(3S)	5340(30)	671(13)	9811(13)	86(8)
C(4S)	6470(40)	570(20)	10078(19)	158(16)
C(5S)	7900(40)	3039(17)	4398(17)	120(12)
C(6S)	8900(40)	2870(20)	4727(19)	156(16)

N(1S)	4450(20)	2220(12)	1377(11)	95(7)
N(2S)	4510(30)	784(15)	9668(14)	132(11)
N(3S)	7100(30)	3178(17)	4173(16)	157(13)
C(21)	3730(30)	2762(12)	4318(11)	105(12)
F(25)	2700(30)	2813(17)	4340(14)	143(14)
F(26)	3950(30)	2214(11)	4282(11)	99(9)
F(27)	4420(20)	2867(11)	4794(10)	159(8)
C(21A)	4040(40)	2653(14)	4284(12)	105(12)
F(25A)	4630(40)	2220(18)	4143(19)	79(16)
F(26A)	3140(40)	2350(20)	4295(18)	78(17)
F(27A)	4420(20)	2867(11)	4794(10)	159(8)

[a] U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Bond lengths (in Å) for $(tfepma)_3Ir_2^{0,II}H_2Cl_2 \bullet 3CH_3CN$.

Bond	Distance	Bond	Distance
Ir(1)–P(4)	2.252(4)	C(8)–C(9)	1.43(3)
Ir(1)–P(5)	2.257(4)	C(9)–F(7)	1.28(3)
Ir(1)–P(6)	2.265(4)	C(9)–F(9)	1.33(3)
Ir(1)–P(2)	2.286(4)	C(9)–F(8)	1.34(4)
Ir(1)–Ir(2)	2.7464(9)	C(10)–C(11)	1.49(3)
Ir(2)–P(1)	2.154(4)	C(11)–F(11)	1.31(3)
Ir(2)–P(3)	2.266(4)	C(11)–F(12)	1.31(3)
Ir(2)–Cl(1)	2.440(5)	C(11)–F(10)	1.36(3)
Ir(2)–Cl(2)	2.465(4)	C(12)–C(13)	1.46(4)
P(1)–O(1)	1.582(12)	C(13)–F(14)	1.24(4)
P(1)–O(2)	1.591(12)	C(13)–F(15)	1.34(4)
P(1)–N(1)	1.670(15)	C(13)–F(13)	1.34(3)
P(2)–O(4)	1.600(12)	C(14)–C(15)	1.46(3)
P(2)–O(3)	1.600(13)	C(15)–F(17)	1.28(4)
P(2)–N(1)	1.658(14)	C(15)–F(18)	1.35(4)
P(3)–O(6)	1.613(13)	C(15)–F(16)	1.37(3)
P(3)–O(5)	1.615(13)	C(16)–C(17)	1.45(3)
P(3)–N(2)	1.700(14)	C(17)–F(20)	1.27(3)
P(4)–O(8)	1.601(14)	C(17)–F(21)	1.30(3)
P(4)–O(7)	1.609(14)	C(17)–F(19)	1.31(4)
P(4)–N(2)	1.644(14)	C(18)–C(19)	1.45(2)
P(5)–O(10)	1.571(12)	C(19)–F(23)	1.30(2)
P(5)–O(9)	1.586(13)	C(19)–F(22)	1.31(2)
P(5)–N(3)	1.693(15)	C(19)–F(24)	1.32(2)
P(6)–O(12)	1.573(14)	C(20)–C(21A)	1.47(2)
P(6)–O(11)	1.594(12)	C(20)–C(21)	1.470(19)
P(6)–N(3)	1.686(15)	C(22)–C(23)	1.47(3)
O(1)–C(4)	1.43(2)	C(23)–F(28)	1.30(3)

O(2)–C(6)	1.40(2)	C(23)–F(30)	1.32(3)
O(3)–C(8)	1.41(2)	C(23)–F(29)	1.32(2)
O(4)–C(10)	1.44(2)	C(24)–C(25)	1.53(3)
O(5)–C(12)	1.43(2)	C(25)–F(33)	1.33(3)
O(6)–C(14)	1.43(2)	C(25)–F(31)	1.33(3)
O(7)–C(16)	1.38(2)	C(25)–F(32)	1.33(3)
O(8)–C(18)	1.44(3)	C(26)–C(27)	1.41(3)
O(9)–C(20)	1.39(3)	C(27)–F(35)	1.27(3)
O(10)–C(22)	1.42(2)	C(27)–F(34)	1.30(3)
O(11)–C(24)	1.40(2)	C(27)–F(36)	1.41(3)
O(12)–C(26)	1.40(2)	C(1S)–C(2S)	1.42(4)
N(1)–C(1)	1.51(2)	C(2S)–N(1S)	1.06(3)
N(2)–C(2)	1.48(2)	C(3S)–N(2S)	1.06(4)
N(3)–C(3)	1.43(2)	C(3S)–C(4S)	1.45(5)
C(4)–C(5)	1.49(3)	C(5S)–N(3S)	1.10(5)
C(5)–F(2)	1.31(2)	C(5S)–C(6S)	1.40(5)
C(5)–F(1)	1.32(2)	C(21)–F(25)	1.292(19)
C(5)–F(3)	1.31(3)	C(21)–F(27)	1.317(19)
C(6)–C(7)	1.46(3)	C(21)–F(26)	1.323(19)
C(7)–F(5)	1.31(4)	C(21A)–F(26A)	1.32(2)
C(7)–F(6)	1.32(3)	C(21A)–F(25A)	1.33(2)
C(7)–F(4)	1.34(4)		

Table S4. Bond angles (in deg) for $(tfepma)_3Ir_2^{0,II}H_2Cl_2 \bullet 3CH_3CN$.

Bond Angle	Angle	Bond Angle	Angle
P(4)–Ir(1)–P(5)	104.56(16)	F(5)–C(7)–F(6)	106(3)
P(4)–Ir(1)–P(6)	169.22(17)	F(5)–C(7)–F(4)	105(3)
P(5)–Ir(1)–P(6)	69.13(15)	F(6)–C(7)–F(4)	104(3)
P(4)–Ir(1)–P(2)	95.02(16)	F(5)–C(7)–C(6)	116(3)
P(5)–Ir(1)–P(2)	109.48(16)	F(6)–C(7)–C(6)	113(2)
P(6)–Ir(1)–P(2)	95.37(15)	F(4)–C(7)–C(6)	111(3)
P(4)–Ir(1)–Ir(2)	89.46(11)	O(3)–C(8)–C(9)	109.8(19)
P(5)–Ir(1)–Ir(2)	158.03(12)	F(7)–C(9)–F(9)	109(2)
P(6)–Ir(1)–Ir(2)	94.20(11)	F(7)–C(9)–F(8)	101(3)
P(2)–Ir(1)–Ir(2)	85.53(11)	F(9)–C(9)–F(8)	105(2)
P(1)–Ir(2)–P(3)	100.84(17)	F(7)–C(9)–C(8)	117(2)
P(1)–Ir(2)–Cl(1)	170.26(16)	F(9)–C(9)–C(8)	113(2)
P(3)–Ir(2)–Cl(1)	87.60(17)	F(8)–C(9)–C(8)	110(3)
P(1)–Ir(2)–Cl(2)	86.95(16)	O(4)–C(10)–C(11)	107.8(17)
P(3)–Ir(2)–Cl(2)	99.30(16)	F(11)–C(11)–F(12)	109(2)
Cl(1)–Ir(2)–Cl(2)	86.88(16)	F(11)–C(11)–F(10)	107.5(18)
P(1)–Ir(2)–Ir(1)	93.95(12)	F(12)–C(11)–F(10)	104(2)
P(3)–Ir(2)–Ir(1)	92.61(11)	F(11)–C(11)–C(10)	111(2)
Cl(1)–Ir(2)–Ir(1)	90.48(11)	F(12)–C(11)–C(10)	112.8(19)
Cl(2)–Ir(2)–Ir(1)	167.67(12)	F(10)–C(11)–C(10)	111.3(19)
O(1)–P(1)–O(2)	96.8(7)	O(5)–C(12)–C(13)	106(2)
O(1)–P(1)–N(1)	102.6(7)	F(14)–C(13)–F(15)	108(3)
O(2)–P(1)–N(1)	98.5(7)	F(14)–C(13)–F(13)	109(3)
O(1)–P(1)–Ir(2)	118.5(5)	F(15)–C(13)–F(13)	104(2)
O(2)–P(1)–Ir(2)	119.8(5)	F(14)–C(13)–C(12)	116(3)
N(1)–P(1)–Ir(2)	116.8(5)	F(15)–C(13)–C(12)	112(3)
O(4)–P(2)–O(3)	101.5(7)	F(13)–C(13)–C(12)	108(3)

O(4)–P(2)–N(1)	106.5(7)	O(6)–C(14)–C(15)	108.1(18)
O(3)–P(2)–N(1)	95.9(7)	F(17)–C(15)–F(18)	106(3)
O(4)–P(2)–Ir(1)	111.2(4)	F(17)–C(15)–F(16)	107(2)
O(3)–P(2)–Ir(1)	123.7(5)	F(18)–C(15)–F(16)	106(3)
N(1)–P(2)–Ir(1)	115.6(5)	F(17)–C(15)–C(14)	116(3)
O(6)–P(3)–O(5)	100.9(7)	F(18)–C(15)–C(14)	112(3)
O(6)–P(3)–N(2)	105.6(7)	F(16)–C(15)–C(14)	109(2)
O(5)–P(3)–N(2)	94.8(7)	O(7)–C(16)–C(17)	110.3(19)
O(6)–P(3)–Ir(2)	115.4(5)	F(20)–C(17)–F(21)	111(3)
O(5)–P(3)–Ir(2)	121.5(5)	F(20)–C(17)–F(19)	102(3)
N(2)–P(3)–Ir(2)	115.5(5)	F(21)–C(17)–F(19)	101(3)
O(8)–P(4)–O(7)	97.0(7)	F(20)–C(17)–C(16)	116(3)
O(8)–P(4)–N(2)	100.3(7)	F(21)–C(17)–C(16)	115(2)
O(7)–P(4)–N(2)	103.7(7)	F(19)–C(17)–C(16)	110(3)
O(8)–P(4)–Ir(1)	117.2(5)	O(8)–C(18)–C(19)	112(2)
O(7)–P(4)–Ir(1)	115.2(5)	F(23)–C(19)–F(22)	110(3)
N(2)–P(4)–Ir(1)	119.9(5)	F(23)–C(19)–F(24)	102(3)
O(10)–P(5)–O(9)	96.1(6)	F(22)–C(19)–F(24)	116(4)
O(10)–P(5)–N(3)	109.1(7)	F(23)–C(19)–C(18)	110(3)
O(9)–P(5)–N(3)	104.2(7)	F(22)–C(19)–C(18)	112(3)
O(10)–P(5)–Ir(1)	124.9(5)	F(24)–C(19)–C(18)	107(3)
O(9)–P(5)–Ir(1)	124.8(5)	O(9)–C(20)–C(21A)	108(2)
N(3)–P(5)–Ir(1)	95.8(5)	O(9)–C(20)–C(21)	109(2)
O(12)–P(6)–O(11)	99.6(7)	C(21A)–C(20)–C(21)	19(2)
O(12)–P(6)–N(3)	109.2(8)	O(10)–C(22)–C(23)	108.8(16)
O(11)–P(6)–N(3)	104.8(7)	F(28)–C(23)–F(30)	109(2)
O(12)–P(6)–Ir(1)	117.6(5)	F(28)–C(23)–F(29)	106.7(18)
O(11)–P(6)–Ir(1)	128.4(5)	F(30)–C(23)–F(29)	108.6(19)
N(3)–P(6)–Ir(1)	95.7(5)	F(28)–C(23)–C(22)	110.4(19)
C(4)–O(1)–P(1)	127.4(11)	F(30)–C(23)–C(22)	113.1(18)

C(6)–O(2)–P(1)	123.3(12)	F(29)–C(23)–C(22)	109.3(19)
C(8)–O(3)–P(2)	123.8(13)	O(11)–C(24)–C(25)	107.5(17)
C(10)–O(4)–P(2)	122.8(11)	F(33)–C(25)–F(31)	109(2)
C(12)–O(5)–P(3)	122.3(12)	F(33)–C(25)–F(32)	108(2)
C(14)–O(6)–P(3)	125.1(13)	F(31)–C(25)–F(32)	109(2)
C(16)–O(7)–P(4)	126.3(12)	F(33)–C(25)–C(24)	111.5(18)
C(18)–O(8)–P(4)	119.8(15)	F(31)–C(25)–C(24)	110(2)
C(20)–O(9)–P(5)	125.5(12)	F(32)–C(25)–C(24)	110(2)
C(22)–O(10)–P(5)	127.7(11)	O(12)–C(26)–C(27)	113(2)
C(24)–O(11)–P(6)	121.1(11)	F(35)–C(27)–F(34)	107(2)
C(26)–O(12)–P(6)	126.3(13)	F(35)–C(27)–C(26)	117(2)
C(1)–N(1)–P(2)	125.0(12)	F(34)–C(27)–C(26)	116(2)
C(1)–N(1)–P(1)	118.0(11)	F(35)–C(27)–F(36)	105(2)
P(2)–N(1)–P(1)	116.5(8)	F(34)–C(27)–F(36)	100(2)
C(2)–N(2)–P(4)	117.9(11)	C(26)–C(27)–F(36)	109(2)
C(2)–N(2)–P(3)	122.8(11)	N(1S)–C(2S)–C(1S)	174(3)
P(4)–N(2)–P(3)	119.2(8)	N(2S)–C(3S)–C(4S)	172(4)
C(3)–N(3)–P(6)	130.3(13)	N(3S)–C(5S)–C(6S)	175(5)
C(3)–N(3)–P(5)	130.9(13)	F(25)–C(21)–F(27)	116(3)
P(6)–N(3)–P(5)	98.8(8)	F(25)–C(21)–F(26)	108(3)
O(1)–C(4)–C(5)	107.7(15)	F(27)–C(21)–F(26)	97(2)
F(2)–C(5)–F(1)	108.1(18)	F(25)–C(21)–C(20)	112(3)
F(2)–C(5)–F(3)	107(2)	F(27)–C(21)–C(20)	111(2)
F(1)–C(5)–F(3)	107.5(18)	F(26)–C(21)–C(20)	112(3)
F(2)–C(5)–C(4)	112.2(17)	F(26A)–C(21A)–F(25A)	95(4)
F(1)–C(5)–C(4)	109.2(19)	F(26A)–C(21A)–C(20)	119(4)
F(3)–C(5)–C(4)	112.2(17)	F(25A)–C(21A)–C(20)	107(3)
O(2)–C(6)–C(7)	108.4(18)		

Table S5. Anisotropic thermal displacement parameters (Å^2 × 10^3) for $(tfepma)_3Ir_2^{0,II}H_2Cl_2$•$3CH_3CN$.

Atom	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	21(1)	24(1)	36(1)	0(1)	7(1)	–2(1)
Ir(2)	21(1)	25(1)	37(1)	–1(1)	6(1)	–3(1)
Cl(1)	48(3)	42(3)	42(3)	–6(2)	12(2)	–10(2)
Cl(2)	44(3)	29(2)	60(3)	–6(2)	14(2)	–14(2)
P(1)	24(2)	33(2)	35(2)	2(2)	7(2)	0(2)
P(2)	25(2)	28(2)	35(2)	–3(2)	3(2)	0(2)
P(3)	24(2)	26(2)	53(3)	–7(2)	17(2)	–6(2)
P(4)	16(2)	32(2)	54(3)	0(2)	10(2)	–5(2)
P(5)	33(2)	29(2)	40(3)	2(2)	9(2)	2(2)
P(6)	21(2)	26(2)	36(2)	4(2)	3(2)	2(2)
O(1)	28(7)	52(8)	44(7)	2(6)	8(5)	–10(6)
O(2)	40(7)	38(7)	41(7)	15(6)	2(5)	4(6)
O(3)	49(8)	33(7)	63(9)	–11(6)	12(6)	–4(6)
O(4)	33(6)	41(7)	27(6)	0(5)	–2(5)	1(5)
O(5)	39(7)	47(8)	71(9)	–9(7)	25(6)	5(6)
O(6)	38(7)	28(6)	66(9)	14(6)	15(6)	12(5)
O(7)	43(8)	38(7)	58(8)	–8(6)	18(6)	–1(6)
O(8)	45(8)	33(7)	77(10)	–8(7)	22(7)	0(6)
O(9)	57(8)	34(7)	48(8)	–2(6)	11(6)	–13(6)
O(10)	39(7)	7(5)	67(8)	6(5)	14(6)	5(5)
O(11)	16(6)	42(7)	69(9)	15(7)	7(5)	6(5)
O(12)	43(8)	42(8)	67(9)	11(7)	13(6)	17(6)
N(1)	35(8)	38(8)	32(8)	2(6)	12(6)	–1(6)
N(2)	24(8)	25(7)	55(9)	–3(7)	8(6)	4(6)
N(3)	38(9)	35(9)	53(10)	7(7)	6(7)	7(7)
C(1)	52(13)	55(13)	45(12)	–1(10)	16(9)	–8(10)
C(2)	66(14)	36(11)	60(13)	14(9)	35(11)	7(10)
C(3)	31(10)	17(8)	78(14)	–4(9)	4(9)	10(7)

C(4)	17(9)	33(10)	59(12)	12(8)	14(8)	5(7)
C(5)	23(11)	53(14)	102(19)	–3(13)	20(11)	–8(10)
C(6)	77(15)	32(11)	52(13)	12(9)	9(11)	4(10)
C(7)	170(30)	50(17)	70(20)	11(15)	0(20)	–14(19)
C(8)	120(20)	34(11)	39(12)	1(9)	–18(12)	–8(12)
C(9)	100(20)	55(16)	62(16)	–17(13)	–14(15)	5(15)
C(10)	31(11)	53(12)	55(12)	9(10)	–9(9)	4(9)
C(11)	50(14)	67(16)	59(15)	–3(12)	–9(11)	2(12)
C(12)	49(13)	31(11)	102(18)	–9(11)	19(12)	6(10)
C(13)	120(30)	62(18)	110(30)	–37(18)	40(20)	–1(18)
C(14)	36(12)	49(13)	98(18)	18(12)	12(11)	4(10)
C(15)	74(19)	80(20)	120(30)	34(19)	40(17)	45(17)
C(16)	56(13)	74(15)	34(11)	–9(10)	19(9)	–25(11)
C(17)	90(20)	110(30)	51(17)	1(17)	23(14)	–12(18)
C(22)	45(12)	36(11)	51(12)	6(9)	–8(9)	–22(9)
C(23)	62(15)	33(12)	81(18)	–5(11)	21(13)	–15(10)
C(24)	33(11)	56(13)	47(12)	13(10)	–2(8)	–2(9)
C(25)	48(15)	110(20)	55(15)	19(15)	–4(11)	–31(15)
C(26)	73(16)	57(14)	80(17)	11(12)	40(13)	3(12)
C(27)	90(20)	60(16)	67(17)	9(13)	43(15)	13(14)
F(1)	32(7)	99(11)	129(13)	26(9)	26(7)	–12(7)
F(2)	60(8)	45(8)	140(13)	20(8)	31(8)	–13(6)
F(3)	94(11)	95(11)	85(10)	–7(9)	63(9)	–10(9)
F(4)	250(30)	94(13)	75(11)	25(10)	78(14)	4(15)
F(5)	180(20)	115(15)	72(11)	26(10)	–42(12)	–16(14)
F(6)	190(20)	62(10)	114(14)	45(10)	16(13)	–29(11)
F(7)	165(19)	97(14)	128(16)	–4(12)	–82(15)	–10(13)
F(8)	220(30)	180(20)	115(16)	–88(16)	49(17)	10(20)
F(9)	220(20)	71(12)	126(16)	–32(11)	–32(15)	–59(14)
F(10)	51(8)	105(13)	105(12)	0(9)	–14(7)	–28(8)
F(11)	57(9)	120(13)	111(12)	23(10)	–34(8)	14(9)

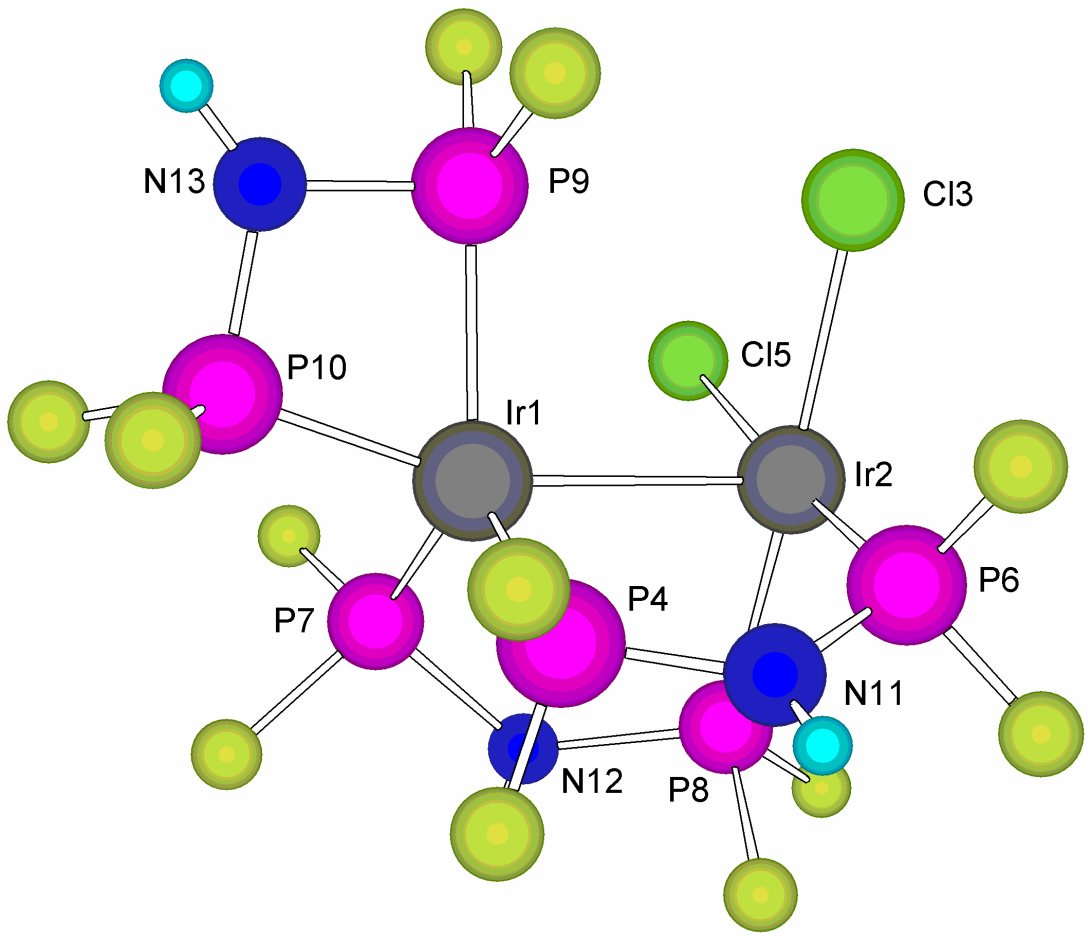
F(12)	51(8)	128(14)	108(12)	–23(10)	10(8)	27(9)
F(13)	126(17)	140(18)	290(30)	–170(20)	59(18)	–46(14)
F(14)	250(30)	200(30)	81(14)	–31(16)	60(17)	30(20)
F(15)	87(12)	81(11)	173(18)	–62(11)	42(11)	12(9)
F(16)	107(14)	154(17)	165(18)	81(15)	44(12)	95(13)
F(17)	106(14)	79(12)	220(20)	73(14)	52(14)	21(11)
F(18)	126(16)	180(20)	109(15)	55(15)	10(12)	79(15)
F(19)	220(30)	160(20)	83(13)	21(14)	60(14)	–57(19)
F(20)	170(20)	200(20)	56(10)	–32(12)	41(11)	–67(17)
F(21)	84(13)	310(30)	87(13)	–37(16)	51(10)	–5(17)
F(28)	49(8)	97(12)	144(14)	8(10)	32(9)	–25(8)
F(29)	95(11)	30(7)	139(13)	7(7)	0(9)	–36(7)
F(30)	98(11)	64(9)	85(11)	–7(8)	–8(8)	–35(8)
F(31)	83(11)	146(16)	92(12)	–9(11)	–14(9)	–59(11)
F(32)	34(8)	121(14)	160(17)	22(12)	–1(8)	–16(9)
F(33)	77(10)	93(11)	116(12)	39(10)	–5(8)	–52(9)
F(34)	190(20)	59(10)	134(15)	7(10)	105(14)	–17(11)
F(35)	131(14)	106(12)	103(12)	20(10)	78(11)	63(11)
F(36)	120(15)	149(18)	87(12)	0(11)	26(11)	4(13)

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

Table S6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $(tfepma)_3Ir_2^{0,II}H_2Cl_2 \bullet 3CH_3CN$.

Atom	x	y	z	U_{eq}
H(1A)	2722	4783	355	75
H(1B)	3370	4193	468	75
H(1C)	4032	4782	526	75
H(2A)	–544	4928	2446	76
H(2B)	–92	5435	2870	76
H(2C)	–132	4799	3107	76
H(3A)	5665	2472	2425	64
H(3B)	5463	2437	3069	64
H(3C)	6374	2860	2904	64
H(4A)	6097	4873	1695	42
H(4B)	5946	5444	2045	42
H(6A)	4030	6296	1315	65
H(6B)	2784	6482	1326	65
H(8A)	1479	3167	1342	79
H(8B)	2606	2837	1319	79
H(10A)	1035	4358	566	58
H(10B)	1017	4972	861	58
H(12A)	2198	6685	2816	72
H(12B)	3063	6285	3216	72
H(14A)	187	6229	2193	73
H(14B)	–378	5725	1791	73
H(16A)	1937	4855	3788	64
H(16B)	2752	4338	4000	64
H(18A)	349	3370	3074	110
H(18B)	1020	3113	2615	110
H(20A)	3851	3496	3882	78
H(20B)	4842	3063	3853	78
H(22A)	3138	1978	2912	55

H(22B)	3666	1888	2349	55
H(24A)	6185	3951	3566	56
H(24B)	5550	4513	3304	56
H(26A)	5783	3009	1614	80
H(26B)	6715	3448	1886	80
H(1S1)	4078	992	1256	143
H(1S2)	4131	1200	623	143
H(1S3)	3028	1284	880	143
H(4S1)	6965	810	9900	237
H(4S2)	6658	167	10030	237
H(4S3)	6562	657	10485	237
H(6S1)	8767	2706	5087	234
H(6S2)	9389	3201	4807	234
H(6S3)	9254	2584	4519	234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Cl5
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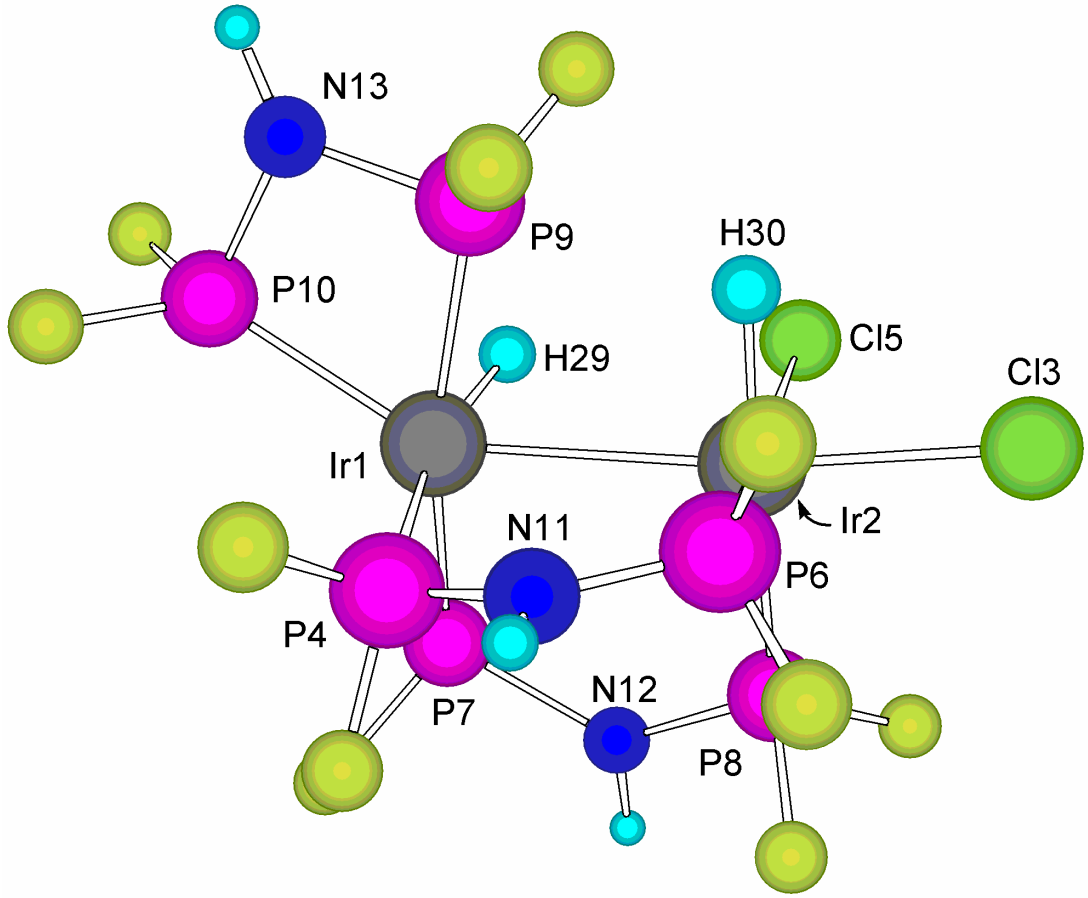
Ir2
P6
P7
P4
N11
N12
P8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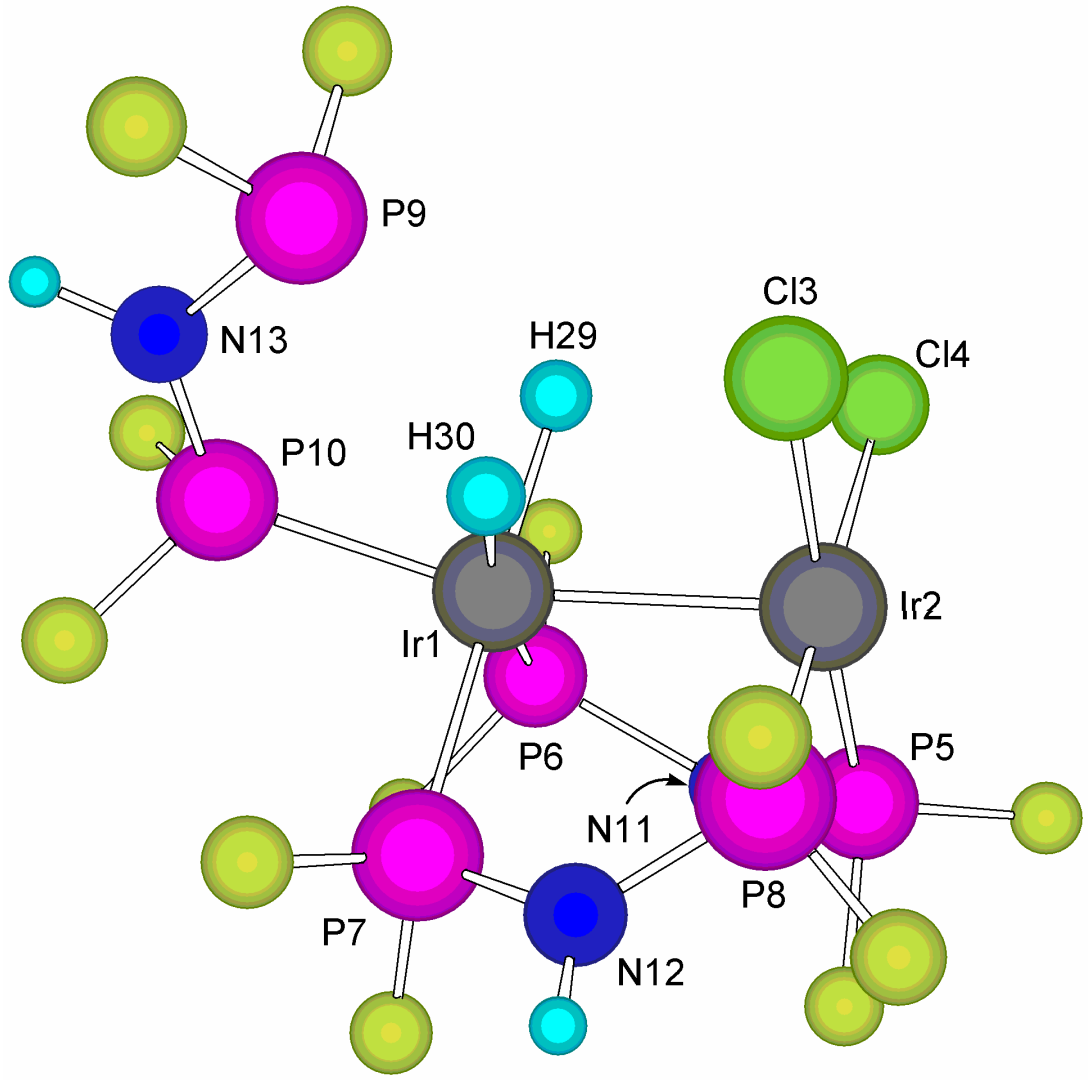
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Ir2
Ir1
P6
P5
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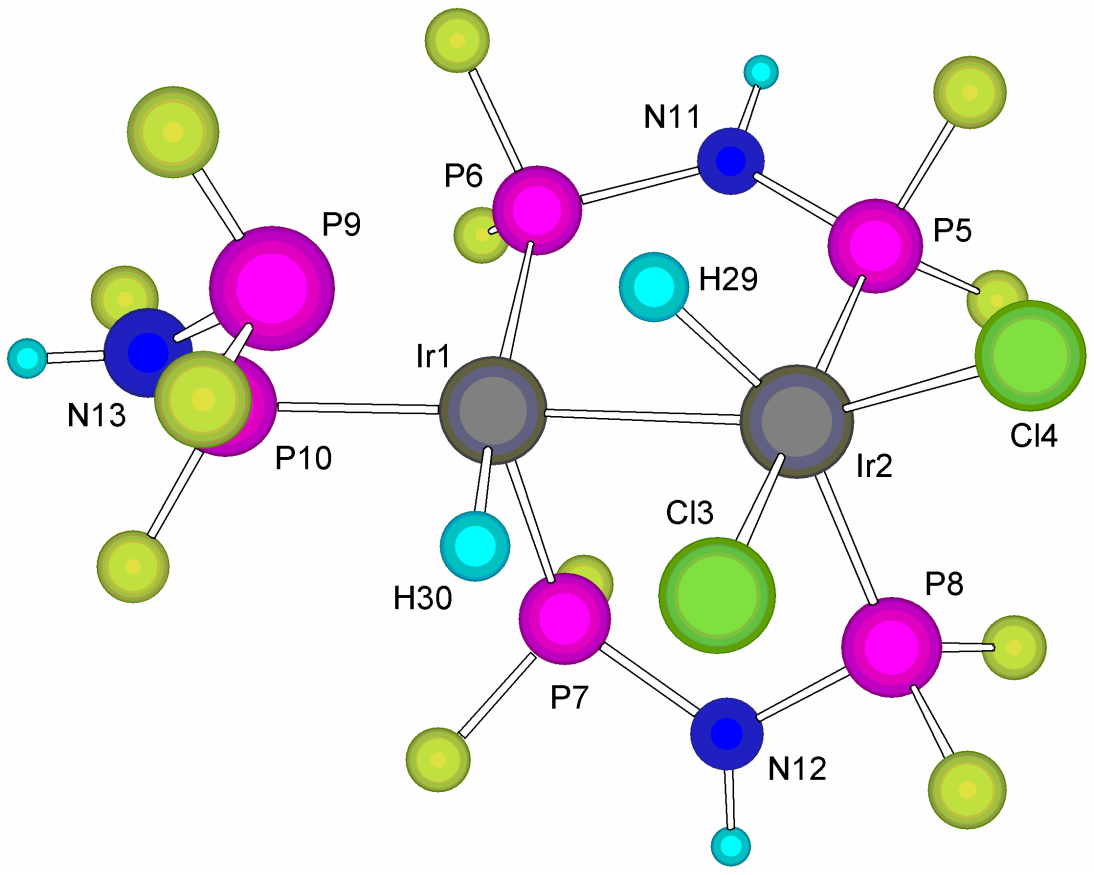
P7
N12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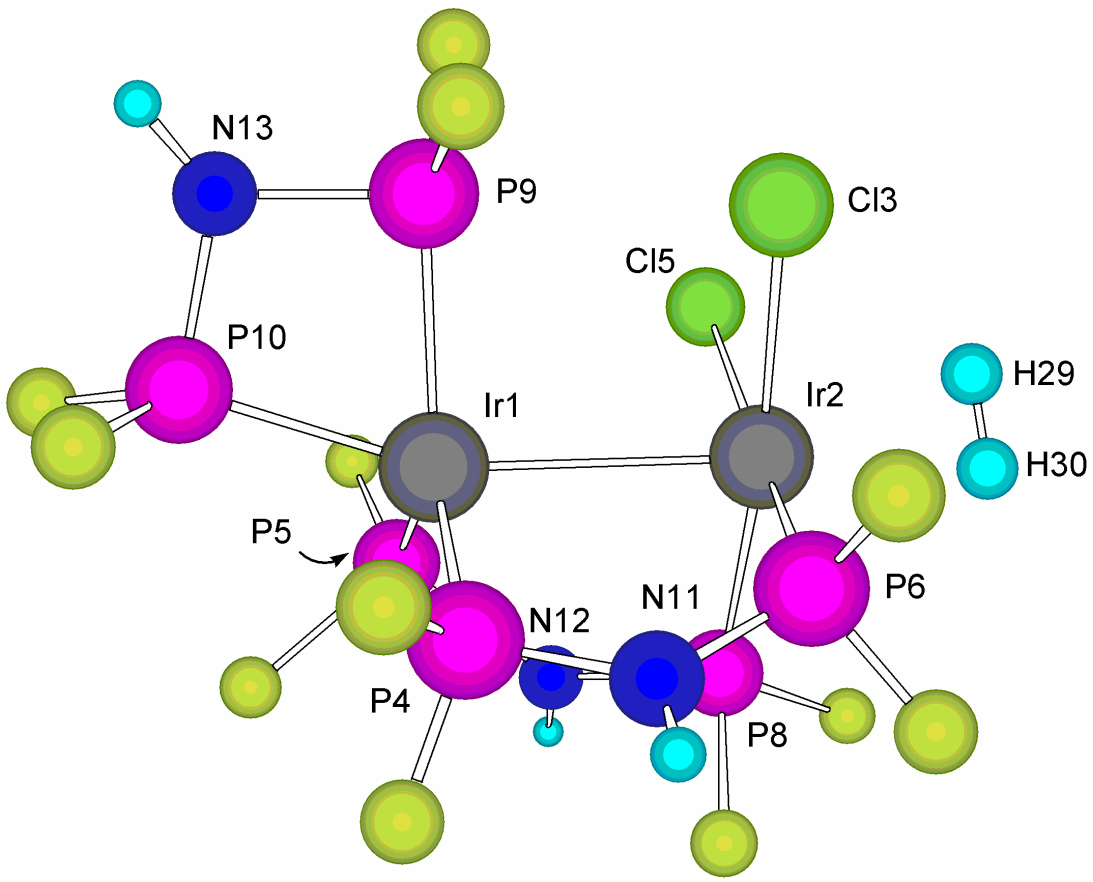
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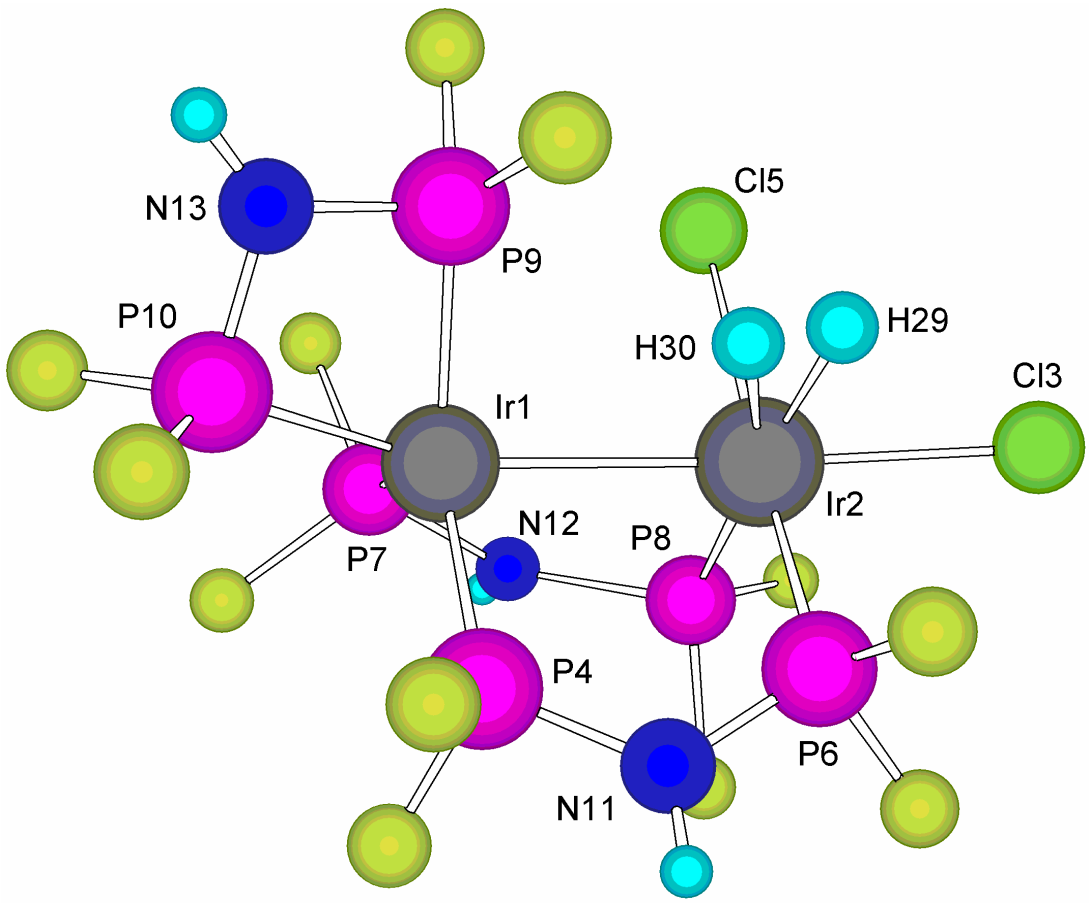
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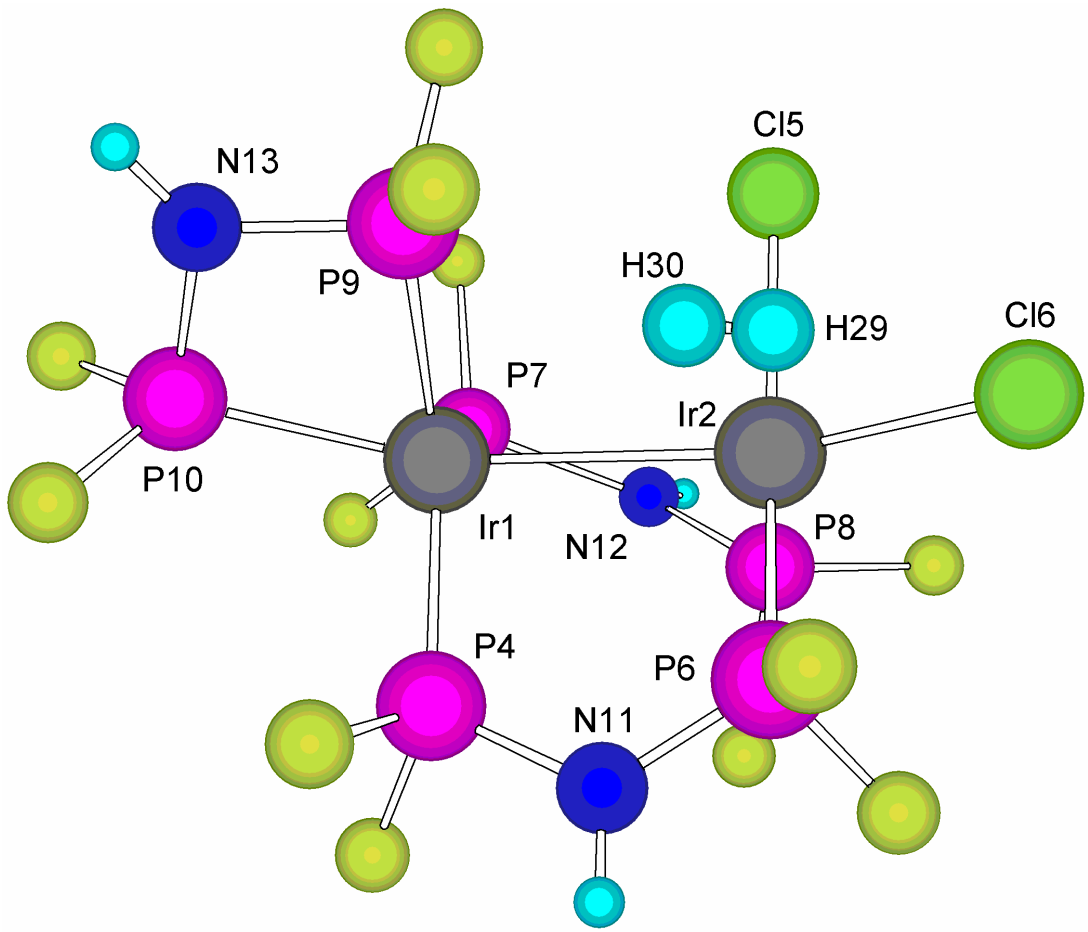
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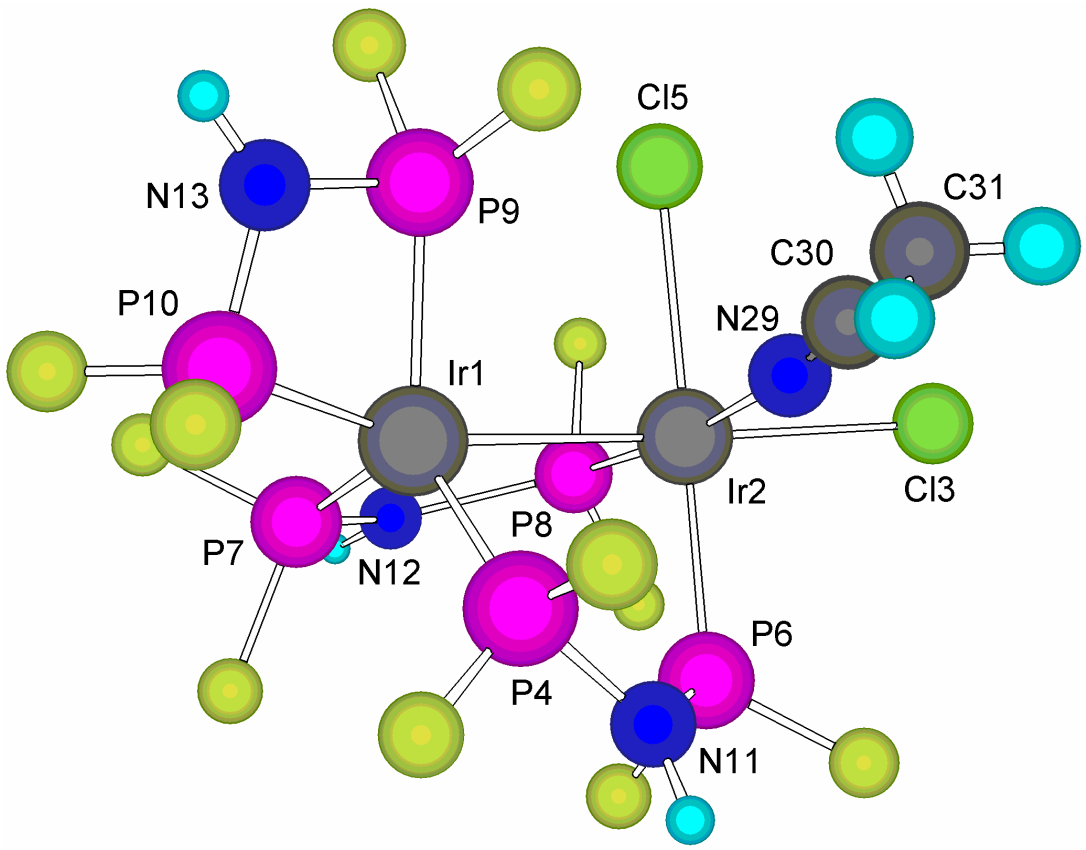
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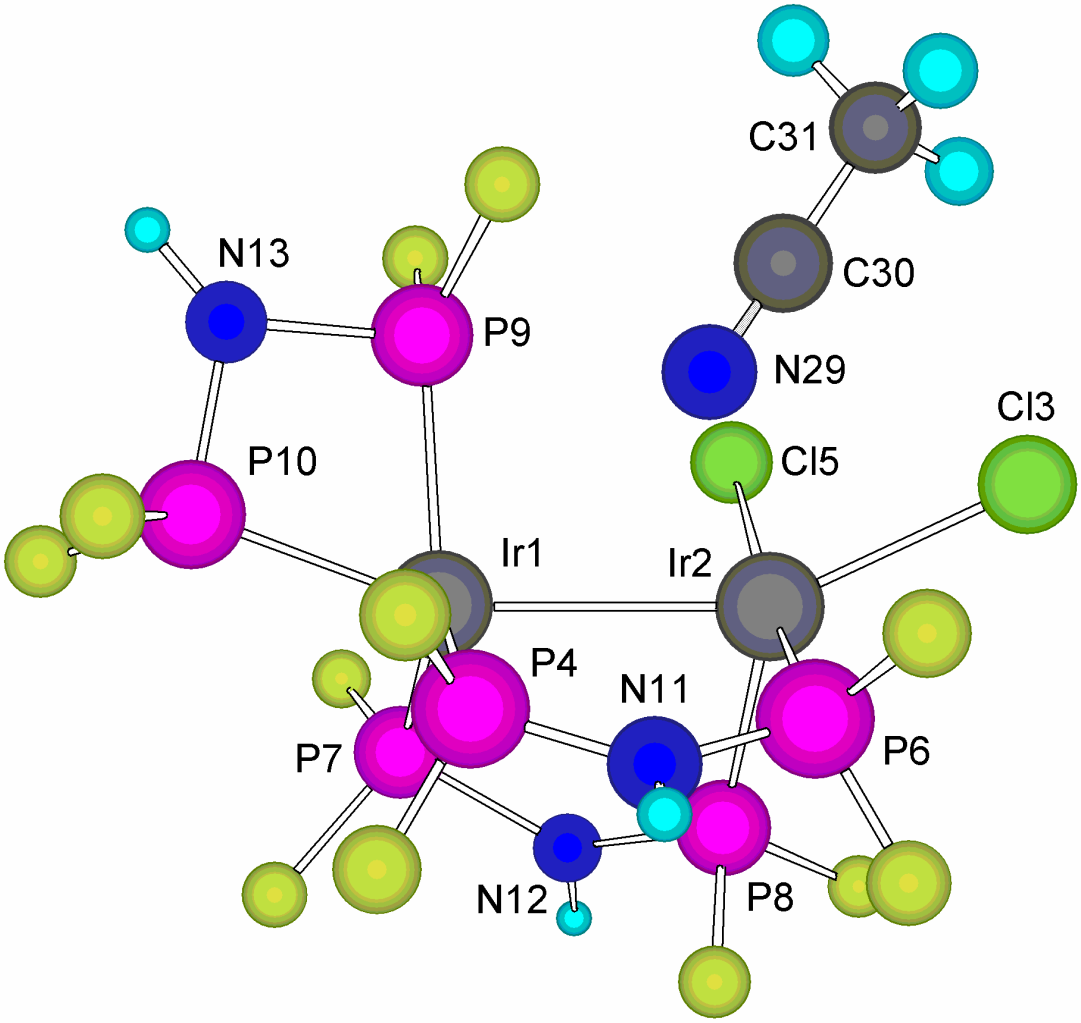
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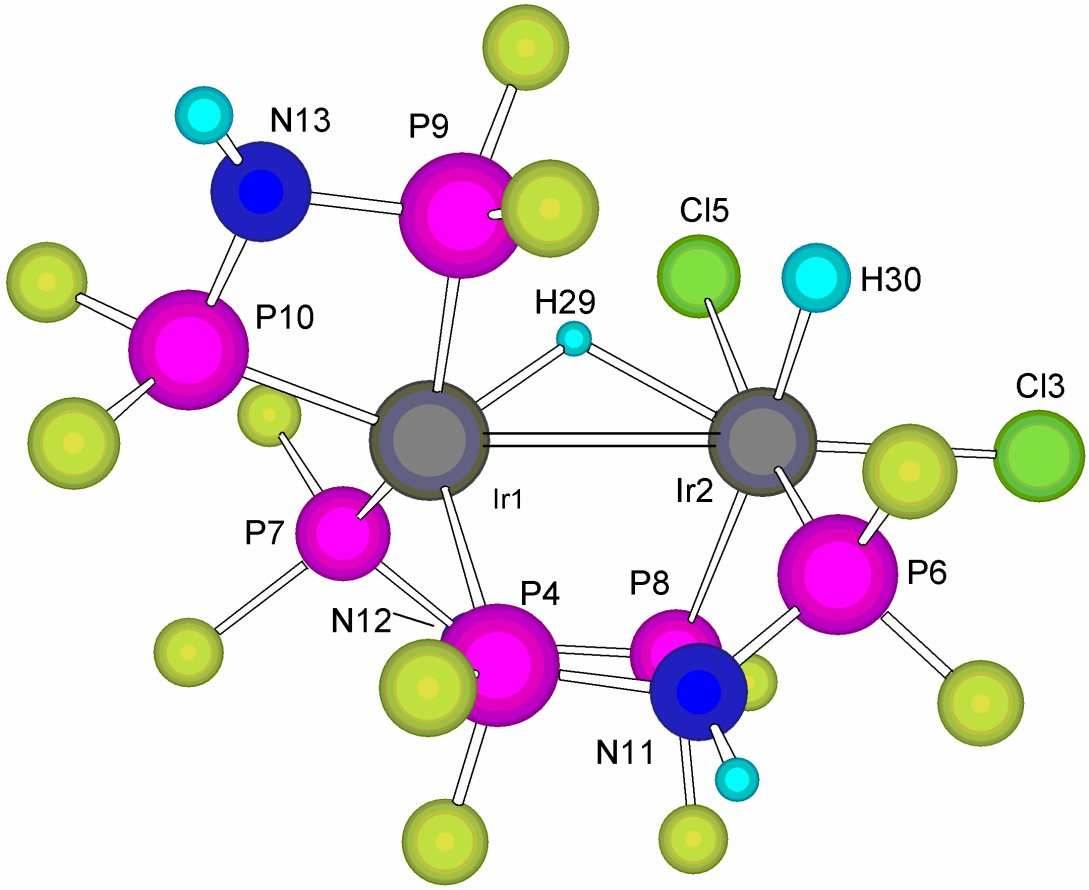
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