CALIFORNIA INSTITUTE OF TECHNOLOGY
BECKMAN INSTITUTE
X-RAY CRYSTALLOGRAPHY LABORATORY

Date 12 March 2010

Crystal Structure Analysis of:

1-Ir(dmap)$_2$

(shown below)

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Account Number: HGB.BP-1-BP.AMOCO

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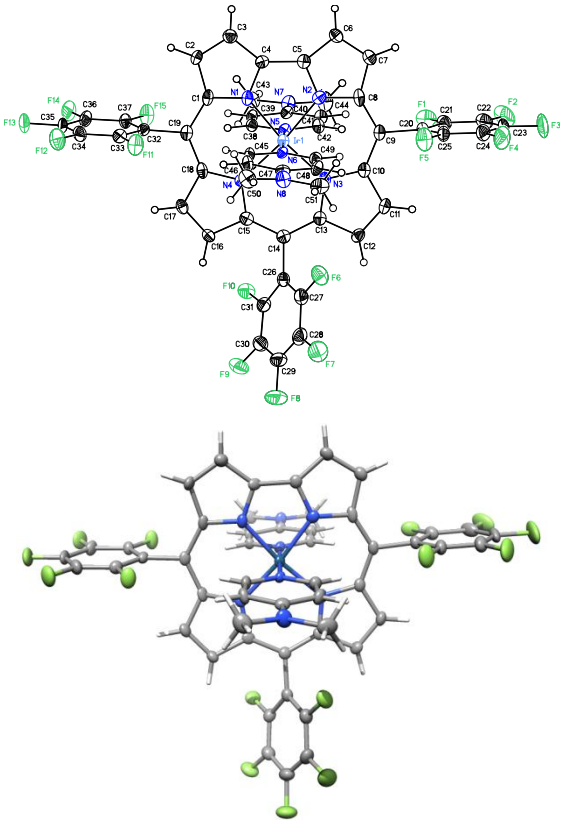


1-Ir(dmap)$_2$

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and have been placed on hold pending further instructions from me. The deposition number is 769414. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 769414".

Table C-4-1. Crystal data and structure refinement for **1-Ir(dmap)$_2$** (CCDC 769414)

Empirical formula	$C_{51}H_{28}F_{15}N_8Ir \bullet 0.748(C_6H_{12})$
Formula weight	1292.78
Crystallization solvent	Dichloromethane/hexanes
Crystal habit	Blade
Crystal size	0.21 x 0.06 x 0.03 mm^3
Crystal color	Dichroic - green/red

Data Collection

Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 Å MoKa	
Data collection temperature	100(2) K	
q range for 9914 reflections used in lattice determination	2.19 to 29.48°	
Unit cell dimensions	a = 10.9258(5) Å	a= 70.957(2)°
	b = 14.9693(7) Å	b= 78.529(2)°
	c = 17.7416(8) Å	g = 69.831(2)°
Volume	2562.5(2) $Å^3$	
Z	2	
Crystal system	Triclinic	
Space group	P-1	
Density (calculated)	1.676 Mg/m^3	
F(000)	1276	
q range for data collection	1.22 to 30.41°	
Completeness to q = 30.41°	88.1 %	

Index ranges	$-14 \leq h \leq 15$, $-21 \leq k \leq 19$, $-24 \leq l \leq 24$
Data collection scan type	ω scans; 9 settings
Reflections collected	38630
Independent reflections	13679 [R_{int}= 0.0679]
Absorption coefficient	2.708 mm^{-1}
Absorption correction	None
Max. and min. transmission	0.9232 and 0.6002

Table C-3-1 cont.

Structure Solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	13679 / 0 / 705
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.537
Final R indices [I>2s(I), 10722 reflections]	R1 = 0.0488, *w*R2 = 0.0732
R indices (all data)	R1 = 0.0766, *w*R2 = 0.0766
Type of weighting scheme used	Sigma
Weighting scheme used	$w = 1/\sigma^2(Fo^2)$
Max shift/error	0.001
Average shift/error	0.000
Largest diff. peak and hole	3.371 and -2.654 e.Å^{-3}

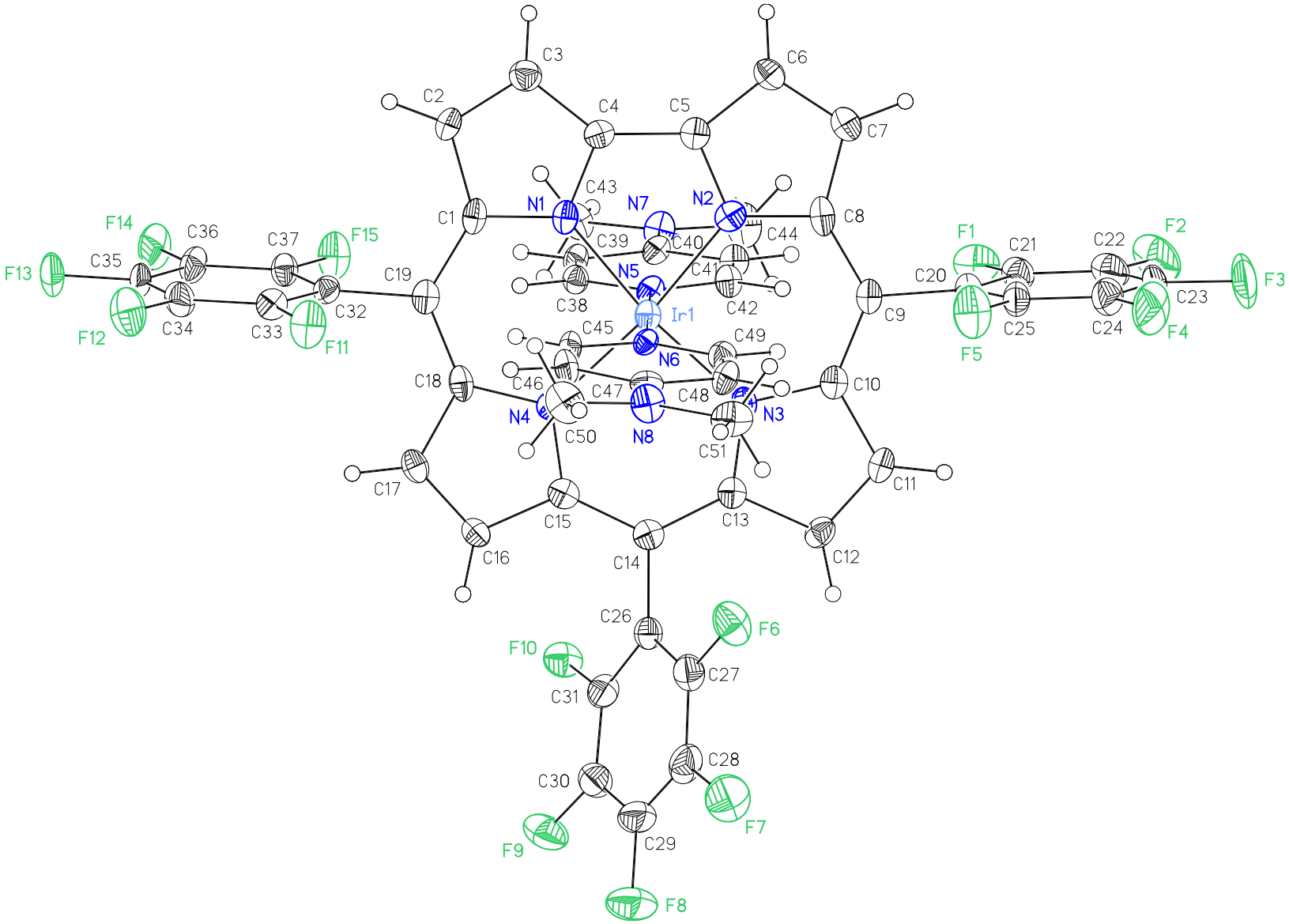
Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The crystal contains methylcyclopentane as a solvent of crystallization. It was refined isotropically and without geometry restraints to a final occupancy of 0.748.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt), etc., and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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C6
C2
C4
C5
C7
C43
N1
N7
N2
C1
C8
C39
C40
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N5
C41
C42
Ir1
C45
C49
N6
C18
C46
C47
C48
C10
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C50
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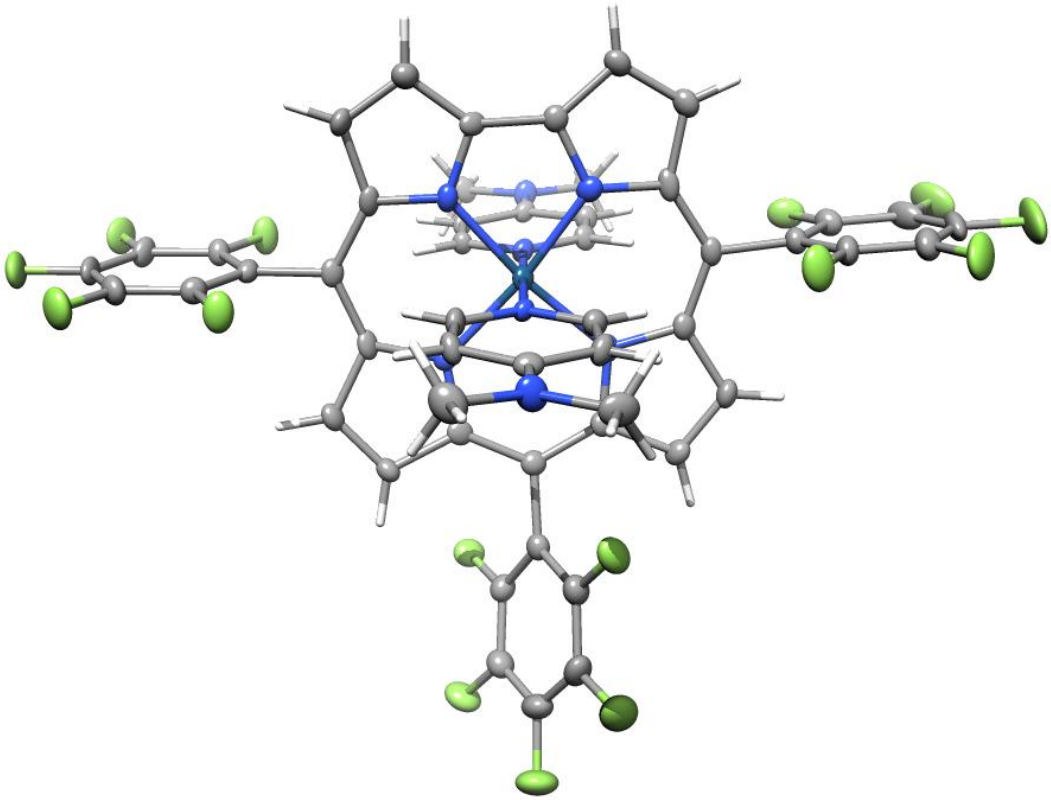
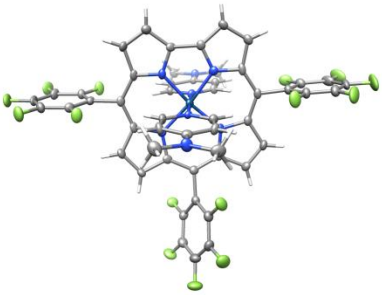
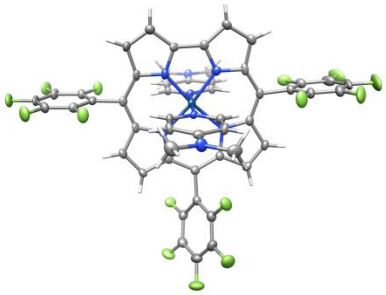
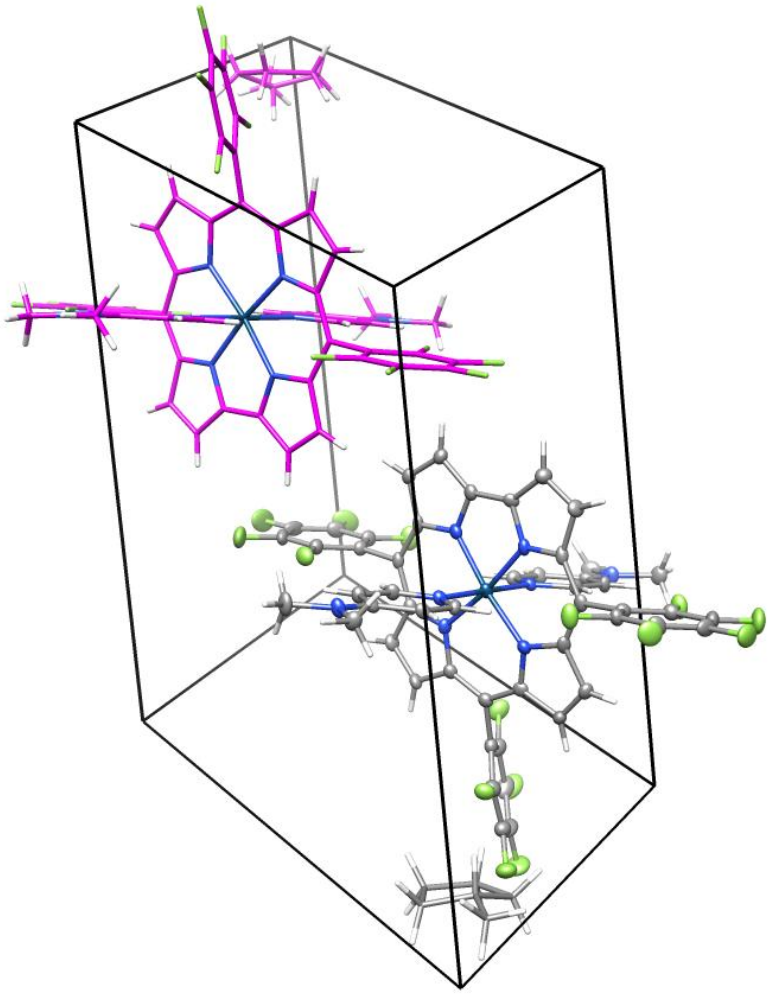








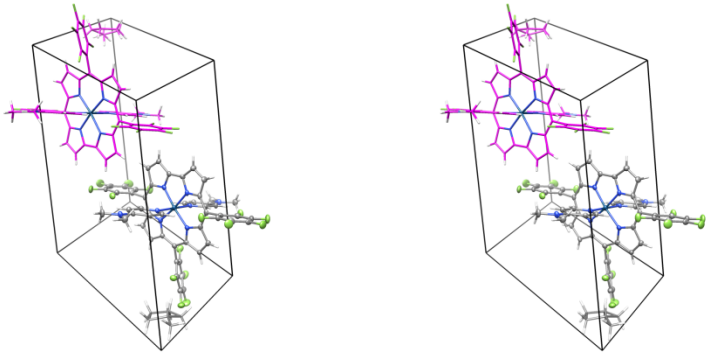


Table C-4-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **1-Ir(dmap)$_2$** (CCDC 769414). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}	Occ
Ir(1)	7000(1)	2834(1)	2994(1)	17(1)	1
F(1)	3846(2)	6561(2)	3060(2)	35(1)	1
F(2)	3388(3)	8523(2)	2824(2)	58(1)	1
F(3)	5420(4)	9302(2)	2369(2)	66(1)	1
F(4)	7894(3)	8117(2)	2156(2)	54(1)	1
F(5)	8346(2)	6172(2)	2403(2)	40(1)	1
F(6)	8868(3)	4004(2)	32(2)	37(1)	1
F(7)	9381(3)	4161(2)	-1530(2)	51(1)	1
F(8)	8163(3)	3395(2)	-2235(2)	51(1)	1
F(9)	6284(3)	2549(2)	-1356(2)	40(1)	1
F(10)	5588(2)	2551(2)	172(1)	29(1)	1
F(11)	10107(2)	-1073(2)	3330(2)	33(1)	1
F(12)	10407(3)	-3040(2)	3732(2)	42(1)	1
F(13)	8311(3)	-3713(2)	4299(2)	40(1)	1
F(14)	5905(3)	-2437(2)	4498(2)	36(1)	1
F(15)	5588(2)	-474(2)	4129(2)	32(1)	1
N(1)	7377(3)	1775(3)	3983(2)	18(1)	1
N(2)	6913(3)	3582(3)	3736(2)	19(1)	1
N(3)	6605(3)	4025(3)	2075(2)	18(1)	1
N(4)	7158(3)	1914(3)	2355(2)	18(1)	1
N(5)	5023(3)	3008(3)	3314(2)	18(1)	1

N(6)	8973(3)	2667(3)	2660(2)	14(1)	1
N(7)	1046(3)	3381(3)	4045(2)	22(1)	1
N(8)	12936(4)	2411(3)	1905(2)	26(1)	1
C(1)	7589(4)	782(3)	4135(3)	19(1)	1
C(2)	7759(4)	358(4)	4984(3)	23(1)	1
C(3)	7591(4)	1125(4)	5289(3)	24(1)	1
C(4)	7340(4)	2021(3)	4661(2)	17(1)	1
C(5)	7047(4)	3073(3)	4520(2)	19(1)	1
C(6)	6835(4)	3802(3)	4926(3)	21(1)	1
C(7)	6555(4)	4719(4)	4371(2)	22(1)	1
C(8)	6600(4)	4593(3)	3596(3)	20(1)	1
C(9)	6377(4)	5229(3)	2819(2)	18(1)	1
C(10)	6388(4)	4976(3)	2118(2)	19(1)	1
C(11)	6236(4)	5614(3)	1314(2)	22(1)	1
C(12)	6397(4)	5041(3)	818(3)	22(1)	1
C(13)	6656(4)	4020(3)	1302(2)	19(1)	1
C(14)	6967(4)	3158(3)	1059(2)	20(1)	1
C(15)	7204(4)	2169(3)	1553(2)	18(1)	1
C(16)	7552(4)	1256(3)	1340(2)	19(1)	1
C(17)	7702(4)	497(3)	2022(2)	21(1)	1
C(18)	7473(4)	891(3)	2687(3)	19(1)	1
C(19)	7630(4)	375(3)	3504(2)	18(1)	1
C(20)	6103(4)	6306(3)	2728(2)	21(1)	1
C(21)	4858(4)	6925(4)	2847(3)	26(1)	1
C(22)	4612(5)	7931(4)	2731(3)	37(1)	1
C(23)	5650(6)	8325(4)	2498(3)	38(1)	1
C(24)	6896(5)	7729(4)	2385(3)	32(1)	1

C(25)	7114(4)	6739(3)	2507(3)	25(1)	1
C(26)	7205(4)	3275(3)	176(2)	21(1)	1
C(27)	8157(5)	3679(4)	-291(3)	28(1)	1
C(28)	8453(5)	3747(4)	-1106(3)	35(1)	1
C(29)	7841(5)	3359(4)	-1461(3)	36(1)	1
C(30)	6903(4)	2947(4)	-1015(3)	29(1)	1
C(31)	6573(4)	2934(3)	-225(3)	26(1)	1
C(32)	7836(4)	-714(3)	3724(2)	19(1)	1
C(33)	9053(4)	-1391(3)	3625(2)	21(1)	1
C(34)	9222(4)	-2398(4)	3818(3)	28(1)	1
C(35)	8156(5)	-2747(3)	4110(3)	27(1)	1
C(36)	6935(4)	-2090(3)	4217(3)	25(1)	1
C(37)	6790(4)	-1096(3)	4027(2)	21(1)	1
C(38)	4543(4)	2235(3)	3564(2)	17(1)	1
C(39)	3235(4)	2330(3)	3809(2)	18(1)	1
C(40)	2322(4)	3262(3)	3804(2)	17(1)	1
C(41)	2848(4)	4061(3)	3547(2)	21(1)	1
C(42)	4161(4)	3908(3)	3311(2)	18(1)	1
C(43)	528(4)	2539(3)	4286(3)	24(1)	1
C(44)	128(4)	4366(4)	3989(3)	30(1)	1
C(45)	9875(4)	1784(3)	2696(2)	20(1)	1
C(46)	11187(4)	1649(3)	2458(2)	21(1)	1
C(47)	11652(4)	2490(3)	2148(2)	20(1)	1
C(48)	10701(4)	3414(3)	2118(2)	21(1)	1
C(49)	9418(4)	3467(3)	2379(2)	21(1)	1
C(50)	13910(4)	1439(4)	2003(3)	33(1)	1
C(51)	13365(4)	3294(4)	1602(3)	30(1)	1

C(61)	1155(16)	-139(13)	718(9)	185(7)	0.748(6)
C(62)	1929(19)	650(14)	470(11)	173(7)	0.748(6)
C(63)	957(15)	1618(12)	205(9)	142(5)	0.748(6)
C(64)	1928(12)	2180(10)	-91(8)	119(5)	0.748(6)
C(65)	3279(11)	1524(10)	-168(7)	106(4)	0.748(6)
C(66)	3299(18)	479(15)	79(10)	194(8)	0.748(6)

Table C-4-3. Selected bond lengths [Å] and angles [°] for **1-Ir(dmap)$_2$** (CCDC 769414)

Ir(1)-N(1)	1.946(3)	N(1)-Ir(1)-N(2)	78.76(15)
Ir(1)-N(2)	1.959(3)	N(1)-Ir(1)-N(3)	172.38(15)
Ir(1)-N(3)	1.968(4)	N(2)-Ir(1)-N(3)	93.62(14)
Ir(1)-N(4)	1.997(3)	N(1)-Ir(1)-N(4)	93.85(14)
Ir(1)-N(5)	2.067(3)	N(2)-Ir(1)-N(4)	172.60(15)
Ir(1)-N(6)	2.069(3)	N(3)-Ir(1)-N(4)	93.76(14)
		N(1)-Ir(1)-N(5)	89.16(13)
		N(2)-Ir(1)-N(5)	87.94(13)
		N(3)-Ir(1)-N(5)	90.74(13)
		N(4)-Ir(1)-N(5)	92.51(13)
		N(1)-Ir(1)-N(6)	91.45(13)
		N(2)-Ir(1)-N(6)	92.37(13)
		N(3)-Ir(1)-N(6)	88.69(13)
		N(4)-Ir(1)-N(6)	87.25(13)
		N(5)-Ir(1)-N(6)	179.36(15)

Table C-4-4. Bond lengths [Å] and angles [°] for **1-Ir(dmap)$_2$** (CCDC 769414)

Ir(1)-N(1)	1.946(3)	N(3)-C(13)	1.364(5)
Ir(1)-N(2)	1.959(3)	N(3)-C(10)	1.386(5)
Ir(1)-N(3)	1.968(4)	N(4)-C(15)	1.343(5)
Ir(1)-N(4)	1.997(3)	N(4)-C(18)	1.392(5)
Ir(1)-N(5)	2.067(3)	N(5)-C(38)	1.342(5)
Ir(1)-N(6)	2.069(3)	N(5)-C(42)	1.351(6)
F(1)-C(21)	1.333(5)	N(6)-C(45)	1.340(6)
F(2)-C(22)	1.338(6)	N(6)-C(49)	1.354(5)
F(3)-C(23)	1.343(6)	N(7)-C(40)	1.341(5)
F(4)-C(24)	1.342(5)	N(7)-C(44)	1.454(6)
F(5)-C(25)	1.335(5)	N(7)-C(43)	1.462(5)
F(6)-C(27)	1.337(5)	N(8)-C(47)	1.359(5)
F(7)-C(28)	1.342(5)	N(8)-C(51)	1.456(5)
F(8)-C(29)	1.336(5)	N(8)-C(50)	1.457(6)
F(9)-C(30)	1.360(5)	C(1)-C(19)	1.427(6)
F(10)-C(31)	1.357(4)	C(1)-C(2)	1.454(6)
F(11)-C(33)	1.343(4)	C(2)-C(3)	1.367(6)
F(12)-C(34)	1.336(5)	C(3)-C(4)	1.417(6)
F(13)-C(35)	1.330(5)	C(4)-C(5)	1.439(6)
F(14)-C(36)	1.340(4)	C(5)-C(6)	1.426(6)
F(15)-C(37)	1.340(5)	C(6)-C(7)	1.377(6)
N(1)-C(4)	1.358(5)	C(7)-C(8)	1.437(6)
N(1)-C(1)	1.363(5)	C(8)-C(9)	1.408(6)
N(2)-C(5)	1.360(5)	C(9)-C(10)	1.410(6)
N(2)-C(8)	1.378(5)	C(9)-C(20)	1.494(6)

C(10)-C(11)	1.439(6)	C(35)-C(36)	1.378(7)
C(11)-C(12)	1.367(6)	C(36)-C(37)	1.372(6)
C(12)-C(13)	1.447(6)	C(38)-C(39)	1.380(5)
C(13)-C(14)	1.404(6)	C(39)-C(40)	1.405(6)
C(14)-C(15)	1.416(6)	C(40)-C(41)	1.409(5)
C(14)-C(26)	1.497(6)	C(41)-C(42)	1.372(5)
C(15)-C(16)	1.441(6)	C(45)-C(46)	1.375(5)
C(16)-C(17)	1.355(6)	C(46)-C(47)	1.421(6)
C(17)-C(18)	1.427(6)	C(47)-C(48)	1.407(6)
C(18)-C(19)	1.416(6)	C(48)-C(49)	1.370(5)
C(19)-C(32)	1.492(6)	C(61)-C(62)	1.583(17)
C(20)-C(21)	1.378(6)	C(62)-C(63)	1.46(2)
C(20)-C(25)	1.396(5)	C(62)-C(66)	1.49(2)
C(21)-C(22)	1.387(7)	C(63)-C(64)	1.489(14)
C(22)-C(23)	1.386(7)	C(64)-C(65)	1.473(16)
C(23)-C(24)	1.364(7)	C(65)-C(66)	1.474(18)
C(24)-C(25)	1.367(6)		
C(26)-C(27)	1.379(5)	N(1)-Ir(1)-N(2)	78.76(15)
C(26)-C(31)	1.385(6)	N(1)-Ir(1)-N(3)	172.38(15)
C(27)-C(28)	1.395(6)	N(2)-Ir(1)-N(3)	93.62(14)
C(28)-C(29)	1.363(7)	N(1)-Ir(1)-N(4)	93.85(14)
C(29)-C(30)	1.361(6)	N(2)-Ir(1)-N(4)	172.60(15)
C(30)-C(31)	1.372(6)	N(3)-Ir(1)-N(4)	93.76(14)
C(32)-C(33)	1.386(6)	N(1)-Ir(1)-N(5)	89.16(13)
C(32)-C(37)	1.388(5)	N(2)-Ir(1)-N(5)	87.94(13)
C(33)-C(34)	1.385(6)	N(3)-Ir(1)-N(5)	90.74(13)
C(34)-C(35)	1.378(6)	N(4)-Ir(1)-N(5)	92.51(13)

N(1)-Ir(1)-N(6)	91.45(13)	C(47)-N(8)-C(50)	120.3(4)
N(2)-Ir(1)-N(6)	92.37(13)	C(51)-N(8)-C(50)	119.2(4)
N(3)-Ir(1)-N(6)	88.69(13)	N(1)-C(1)-C(19)	120.4(4)
N(4)-Ir(1)-N(6)	87.25(13)	N(1)-C(1)-C(2)	105.8(4)
N(5)-Ir(1)-N(6)	179.36(15)	C(19)-C(1)-C(2)	133.8(4)
C(4)-N(1)-C(1)	111.6(4)	C(3)-C(2)-C(1)	107.1(4)
C(4)-N(1)-Ir(1)	118.5(3)	C(2)-C(3)-C(4)	108.8(4)
C(1)-N(1)-Ir(1)	129.8(3)	N(1)-C(4)-C(3)	106.7(4)
C(5)-N(2)-C(8)	113.1(4)	N(1)-C(4)-C(5)	112.3(4)
C(5)-N(2)-Ir(1)	117.7(3)	C(3)-C(4)-C(5)	141.0(4)
C(8)-N(2)-Ir(1)	128.9(3)	N(2)-C(5)-C(6)	105.7(4)
C(13)-N(3)-C(10)	110.8(4)	N(2)-C(5)-C(4)	112.6(4)
C(13)-N(3)-Ir(1)	125.0(3)	C(6)-C(5)-C(4)	141.7(4)
C(10)-N(3)-Ir(1)	123.8(3)	C(7)-C(6)-C(5)	108.1(4)
C(15)-N(4)-C(18)	111.8(4)	C(6)-C(7)-C(8)	108.9(4)
C(15)-N(4)-Ir(1)	124.8(3)	N(2)-C(8)-C(9)	120.1(4)
C(18)-N(4)-Ir(1)	122.4(3)	N(2)-C(8)-C(7)	104.3(4)
C(38)-N(5)-C(42)	116.9(4)	C(9)-C(8)-C(7)	135.6(4)
C(38)-N(5)-Ir(1)	122.0(3)	C(8)-C(9)-C(10)	128.2(4)
C(42)-N(5)-Ir(1)	121.0(3)	C(8)-C(9)-C(20)	115.7(4)
C(45)-N(6)-C(49)	116.3(4)	C(10)-C(9)-C(20)	116.1(4)
C(45)-N(6)-Ir(1)	123.0(3)	N(3)-C(10)-C(9)	125.3(4)
C(49)-N(6)-Ir(1)	120.7(3)	N(3)-C(10)-C(11)	106.1(4)
C(40)-N(7)-C(44)	120.6(4)	C(9)-C(10)-C(11)	128.5(4)
C(40)-N(7)-C(43)	120.7(4)	C(12)-C(11)-C(10)	108.4(4)
C(44)-N(7)-C(43)	118.4(4)	C(11)-C(12)-C(13)	107.8(4)
C(47)-N(8)-C(51)	120.3(4)	N(3)-C(13)-C(14)	124.1(4)

N(3)-C(13)-C(12)	106.7(4)	C(24)-C(23)-C(22)	120.2(5)
C(14)-C(13)-C(12)	129.1(4)	F(4)-C(24)-C(23)	119.9(5)
C(13)-C(14)-C(15)	127.5(4)	F(4)-C(24)-C(25)	120.6(5)
C(13)-C(14)-C(26)	116.8(4)	C(23)-C(24)-C(25)	119.5(4)
C(15)-C(14)-C(26)	115.4(4)	F(5)-C(25)-C(24)	118.1(4)
N(4)-C(15)-C(14)	123.9(4)	F(5)-C(25)-C(20)	119.3(4)
N(4)-C(15)-C(16)	106.1(4)	C(24)-C(25)-C(20)	122.6(4)
C(14)-C(15)-C(16)	130.1(4)	C(27)-C(26)-C(31)	114.8(4)
C(17)-C(16)-C(15)	108.3(4)	C(27)-C(26)-C(14)	121.2(4)
C(16)-C(17)-C(18)	108.7(4)	C(31)-C(26)-C(14)	123.9(4)
N(4)-C(18)-C(19)	126.1(4)	F(6)-C(27)-C(26)	120.5(4)
N(4)-C(18)-C(17)	105.1(4)	F(6)-C(27)-C(28)	116.9(4)
C(19)-C(18)-C(17)	128.6(4)	C(26)-C(27)-C(28)	122.6(4)
C(18)-C(19)-C(1)	127.3(4)	F(7)-C(28)-C(29)	120.3(4)
C(18)-C(19)-C(32)	115.8(4)	F(7)-C(28)-C(27)	119.6(4)
C(1)-C(19)-C(32)	116.9(4)	C(29)-C(28)-C(27)	120.0(4)
C(21)-C(20)-C(25)	116.5(4)	F(8)-C(29)-C(30)	121.5(4)
C(21)-C(20)-C(9)	122.5(4)	F(8)-C(29)-C(28)	119.7(4)
C(25)-C(20)-C(9)	120.9(4)	C(30)-C(29)-C(28)	118.8(4)
F(1)-C(21)-C(20)	119.7(4)	F(9)-C(30)-C(29)	119.8(4)
F(1)-C(21)-C(22)	118.4(4)	F(9)-C(30)-C(31)	119.8(4)
C(20)-C(21)-C(22)	121.9(4)	C(29)-C(30)-C(31)	120.4(4)
F(2)-C(22)-C(23)	120.0(5)	F(10)-C(31)-C(30)	117.1(4)
F(2)-C(22)-C(21)	120.8(5)	F(10)-C(31)-C(26)	119.7(4)
C(23)-C(22)-C(21)	119.2(5)	C(30)-C(31)-C(26)	123.2(4)
F(3)-C(23)-C(24)	120.1(5)	C(33)-C(32)-C(37)	116.6(4)
F(3)-C(23)-C(22)	119.7(5)	C(33)-C(32)-C(19)	122.7(4)

C(37)-C(32)-C(19)	120.7(4)	C(48)-C(47)-C(46)	115.9(4)
F(11)-C(33)-C(34)	118.3(4)	C(49)-C(48)-C(47)	120.3(4)
F(11)-C(33)-C(32)	119.8(4)	N(6)-C(49)-C(48)	123.8(4)
C(34)-C(33)-C(32)	121.9(4)	C(63)-C(62)-C(66)	119.5(16)
F(12)-C(34)-C(35)	119.3(4)	C(63)-C(62)-C(61)	105.9(15)
F(12)-C(34)-C(33)	120.9(4)	C(66)-C(62)-C(61)	124.1(17)
C(35)-C(34)-C(33)	119.8(4)	C(62)-C(63)-C(64)	95.2(13)
F(13)-C(35)-C(36)	120.4(4)	C(65)-C(64)-C(63)	112.2(12)
F(13)-C(35)-C(34)	120.1(4)	C(64)-C(65)-C(66)	110.6(12)
C(36)-C(35)-C(34)	119.5(4)	C(65)-C(66)-C(62)	96.1(15)
F(14)-C(36)-C(37)	121.2(4)		
F(14)-C(36)-C(35)	119.0(4)		
C(37)-C(36)-C(35)	119.8(4)		
F(15)-C(37)-C(36)	118.4(4)		
F(15)-C(37)-C(32)	119.1(4)		
C(36)-C(37)-C(32)	122.4(4)		
N(5)-C(38)-C(39)	123.0(4)		
C(38)-C(39)-C(40)	121.0(4)		
N(7)-C(40)-C(39)	122.7(4)		
N(7)-C(40)-C(41)	122.2(4)		
C(39)-C(40)-C(41)	115.2(4)		
C(42)-C(41)-C(40)	120.5(4)		
N(5)-C(42)-C(41)	123.5(4)		
N(6)-C(45)-C(46)	124.5(4)		
C(45)-C(46)-C(47)	119.3(4)		
N(8)-C(47)-C(48)	121.7(4)		
N(8)-C(47)-C(46)	122.4(4)		

Table C-4-5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **1-Ir(dmap)$_2$** (CCDC 769414). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	137(1)	160(1)	235(1)	-51(1)	-33(1)	-58(1)
F(1)	187(14)	480(20)	352(15)	-146(14)	0(11)	-55(13)
F(2)	510(20)	480(20)	630(20)	-340(18)	-201(16)	256(16)
F(3)	1070(30)	161(19)	780(20)	-163(18)	-410(20)	-17(18)
F(4)	730(20)	380(20)	660(20)	-52(17)	-199(18)	-388(18)
F(5)	233(15)	355(19)	654(19)	-154(16)	-5(14)	-155(13)
F(6)	340(16)	394(19)	472(17)	-201(15)	70(13)	-214(14)
F(7)	540(20)	510(20)	480(18)	-161(17)	220(15)	-296(17)
F(8)	620(20)	630(30)	259(15)	-170(16)	68(14)	-185(18)
F(9)	412(17)	490(20)	367(15)	-224(15)	-104(13)	-90(15)
F(10)	255(14)	377(18)	301(14)	-109(13)	-39(11)	-148(12)
F(11)	162(13)	290(18)	521(17)	-96(14)	-9(12)	-64(12)
F(12)	308(16)	274(18)	574(18)	-165(15)	-55(14)	72(13)
F(13)	600(20)	145(16)	473(17)	-80(14)	-131(15)	-96(14)
F(14)	404(17)	286(18)	484(17)	-58(14)	-38(13)	-256(14)
F(15)	176(13)	246(17)	527(17)	-97(14)	-7(12)	-84(12)
N(1)	116(17)	150(20)	258(19)	-47(16)	-10(14)	-28(15)
N(2)	116(17)	210(20)	211(18)	-45(17)	-13(14)	-18(16)
N(3)	155(18)	160(20)	254(19)	-62(17)	-4(15)	-71(16)
N(4)	140(18)	190(20)	191(18)	-44(16)	-35(14)	-39(16)

N(5)	152(18)	170(20)	195(18)	-19(16)	-29(15)	-65(16)
N(6)	135(18)	140(20)	150(17)	-16(15)	-23(14)	-55(16)
N(7)	127(18)	220(20)	310(20)	-48(18)	-25(15)	-54(17)
N(8)	155(19)	280(30)	350(20)	-100(20)	15(16)	-100(20)
C(1)	110(20)	140(20)	280(20)	-30(20)	20(17)	-52(18)
C(2)	290(30)	160(30)	230(20)	-10(20)	-25(19)	-90(20)
C(3)	250(20)	250(30)	230(20)	-70(20)	-8(19)	-90(20)
C(4)	140(20)	230(30)	190(20)	-43(19)	-23(16)	-105(19)
C(5)	110(20)	210(30)	240(20)	-60(20)	-6(17)	-41(18)
C(6)	160(20)	240(30)	240(20)	-110(20)	12(18)	-51(19)
C(7)	150(20)	230(30)	280(20)	-110(20)	-15(18)	-36(19)
C(8)	90(20)	150(30)	380(30)	-90(20)	-28(18)	-24(18)
C(9)	110(20)	150(20)	280(20)	-60(20)	-3(17)	-36(18)
C(10)	140(20)	180(30)	260(20)	-50(20)	-14(17)	-63(18)
C(11)	220(20)	150(30)	270(20)	-10(20)	-31(18)	-61(19)
C(12)	180(20)	190(30)	210(20)	-20(20)	-32(18)	-10(20)
C(13)	150(20)	190(30)	230(20)	-60(20)	-32(17)	-61(18)
C(14)	160(20)	230(30)	220(20)	-60(20)	-31(17)	-70(19)
C(15)	110(20)	240(30)	220(20)	-80(20)	-2(16)	-89(19)
C(16)	170(20)	200(30)	220(20)	-100(20)	-38(18)	-28(19)
C(17)	180(20)	190(30)	280(20)	-110(20)	-15(18)	-71(19)
C(18)	130(20)	160(30)	320(20)	-80(20)	-38(18)	-67(18)
C(19)	96(19)	180(30)	270(20)	-50(20)	-15(17)	-55(18)
C(20)	210(20)	170(30)	240(20)	-70(20)	-34(18)	-51(19)
C(21)	250(20)	240(30)	280(20)	-100(20)	-60(20)	-10(20)
C(22)	390(30)	300(30)	330(30)	-160(30)	-140(20)	140(20)
C(23)	680(40)	160(30)	330(30)	-80(20)	-200(30)	-90(30)

C(24)	430(30)	250(30)	350(30)	-70(20)	-110(20)	-150(30)
C(25)	290(30)	170(30)	290(20)	-60(20)	-60(20)	-70(20)
C(26)	190(20)	180(30)	250(20)	-60(20)	-20(18)	-34(19)
C(27)	300(30)	240(30)	320(30)	-90(20)	0(20)	-90(20)
C(28)	380(30)	260(30)	330(30)	-50(20)	110(20)	-120(30)
C(29)	450(30)	330(30)	230(20)	-80(20)	20(20)	-60(30)
C(30)	310(30)	270(30)	300(30)	-100(20)	-60(20)	-60(20)
C(31)	270(20)	230(30)	260(20)	-40(20)	-47(19)	-80(20)
C(32)	230(20)	170(30)	190(20)	-29(19)	-62(18)	-68(19)
C(33)	180(20)	230(30)	230(20)	-60(20)	-24(18)	-75(19)
C(34)	290(30)	200(30)	310(20)	-100(20)	-70(20)	30(20)
C(35)	450(30)	120(30)	280(20)	-30(20)	-90(20)	-120(20)
C(36)	280(30)	180(30)	310(20)	-10(20)	-70(20)	-120(20)
C(37)	180(20)	170(30)	260(20)	-60(20)	-52(18)	-33(19)
C(38)	150(20)	150(30)	200(20)	-52(19)	-3(17)	-28(18)
C(39)	180(20)	150(30)	220(20)	-18(19)	-41(18)	-90(19)
C(40)	150(20)	180(30)	190(20)	-17(19)	-30(17)	-69(19)
C(41)	160(20)	200(30)	260(20)	-70(20)	-19(18)	-51(19)
C(42)	140(20)	180(30)	260(20)	-70(20)	-27(18)	-74(19)
C(43)	170(20)	270(30)	340(30)	-130(20)	2(19)	-100(20)
C(44)	110(20)	280(30)	490(30)	-130(30)	0(20)	-20(20)
C(45)	230(20)	130(30)	240(20)	-30(20)	-44(19)	-70(20)
C(46)	180(20)	140(30)	320(20)	-90(20)	-60(19)	-22(19)
C(47)	160(20)	260(30)	180(20)	-60(20)	-36(18)	-70(20)
C(48)	190(20)	170(30)	260(20)	0(20)	-42(18)	-80(20)
C(49)	220(20)	190(30)	220(20)	-50(20)	-9(18)	-80(20)
C(50)	190(30)	370(30)	440(30)	-170(30)	-30(20)	-50(20)

C(51) 200(20) 430(30) 290(20) -100(20) 30(20) -170(20)

CALIFORNIA INSTITUTE OF TECHNOLOGY
BECKMAN INSTITUTE
X-RAY CRYSTALLOGRAPHY LABORATORY

Date 12 March 2010

Crystal Structure Analysis of:

1-Ir(NH_3)$_2$

(shown below)

For Investigator: Theis Brock-Nannestad ext. 6332

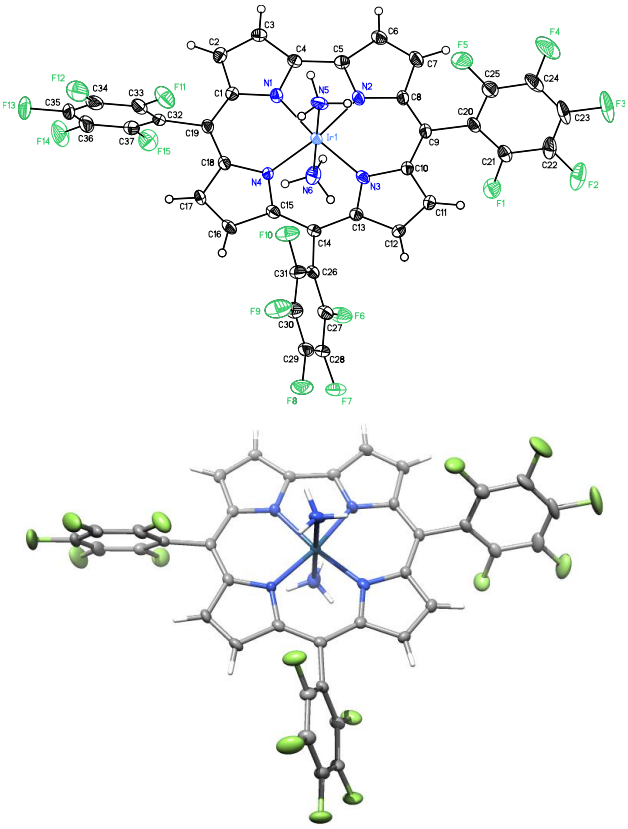
Advisor: H. B. Gray ext. 6500

Account Number: HBG.BP-1-BP.AMOCO

By Michael W. Day 116 Beckman ext. 2734

e-mail: mikeday@caltech.edu

Contents



1-Ir(NH_3)$_2$

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and have been placed on hold pending further instructions from me. The deposition number is 769388. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK, and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 769388".

Table C-5-1. Crystal data and structure refinement for **1-Ir(NH$_3$)$_2$** (CCDC 769388)

Empirical formula	$C_{37}H_{14}F_{15}N_6Ir$	
Formula weight	1019.74	
Crystallization solvent	Dichloromethane/hexanes	
Crystal habit	Fragment	
Crystal size	0.30 x 0.12 x 0.07 mm^3	
Crystal color	Black	

Data Collection

Type of diffractometer	Bruker KAPPA APEX II	
Wavelength	0.71073 Å MoKa	
Data collection temperature	100(2) K	
q range for 9859 reflections used in lattice determination	3.01 to 32.11°	
Unit cell dimensions	a = 17.9079(6) Å	
	b = 7.0034(3) Å	b= 102.528(2)°
	c = 27.0846(10) Å	
Volume	3316.0(2) Å^3	
Z	4	
Crystal system	Monoclinic	
Space group	P $2_1/c$	
Density (calculated)	2.043 Mg/m^3	
F(000)	1960	
Data collection program	Bruker APEX2 v2009.7-0	
q range for data collection	1.16 to 32.14°	

Completeness to q = 32.14°	99.6 %
Index ranges	$-26 \leq h \leq 26, -10 \leq k \leq 10, -40 \leq l \leq 40$
Data collection scan type	ω scans; 11 settings
Data reduction program	Bruker SAINT-Plus v7.66A
Reflections collected	67007
Independent reflections	11625 [R_{int}= 0.0633]
Absorption coefficient	4.153 mm^{-1}
Absorption correction	Gaussian
Max. and min. transmission	0.7532 and 0.5082

Structure Solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 2008)
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 2008)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	11625 / 0 / 534
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.953
Final R indices [I>2s(I), 9482 reflections]	R1 = 0.0374, *w*R2 = 0.0556
R indices (all data)	R1 = 0.0524, *w*R2 = 0.0571
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$

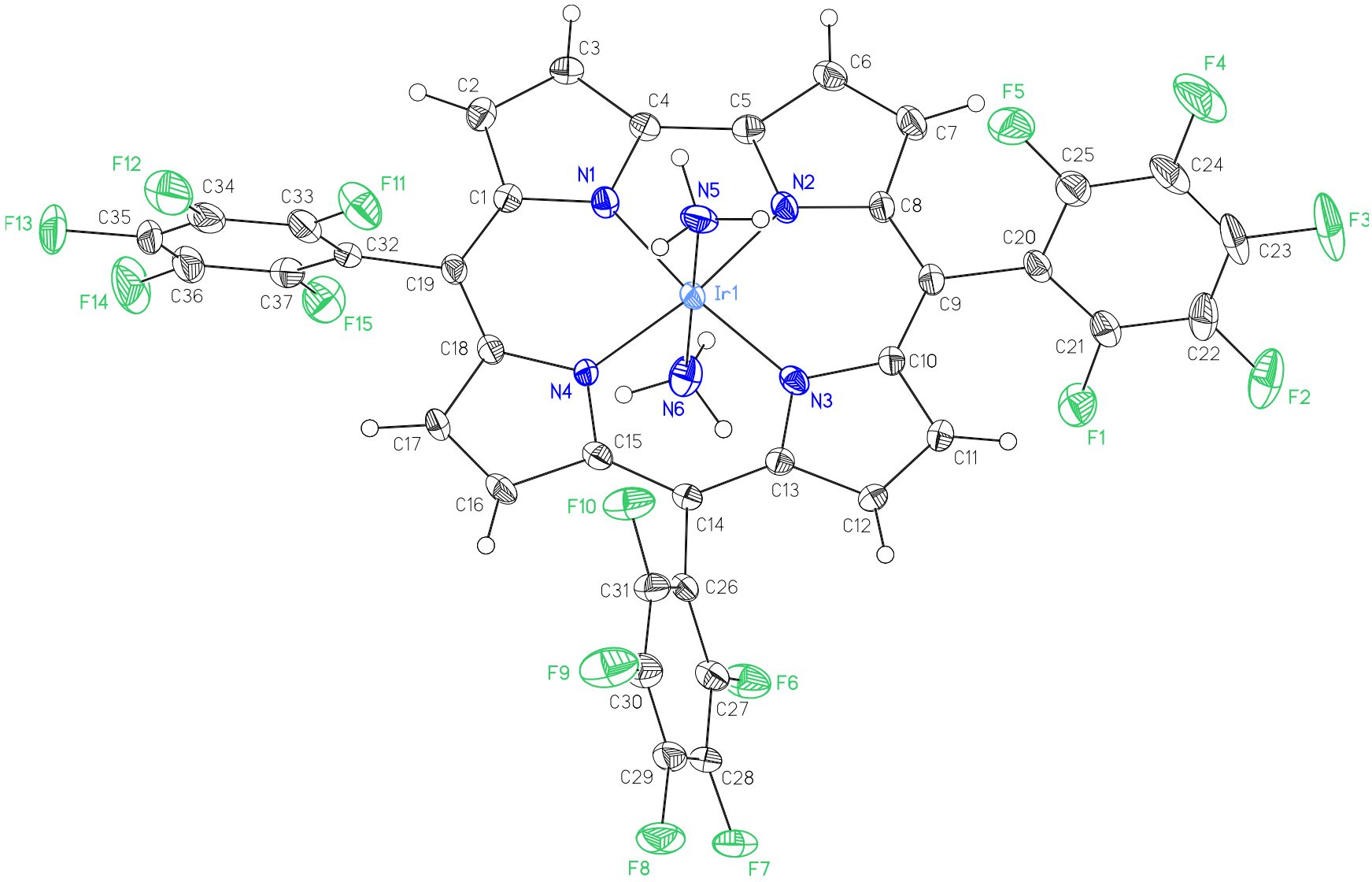
Max shift/error	0.003
Average shift/error	0.000
Largest diff. peak and hole	3.497 and -3.184 e.Å^{-3}

Special Refinement Details

Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt), etc., and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles, and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.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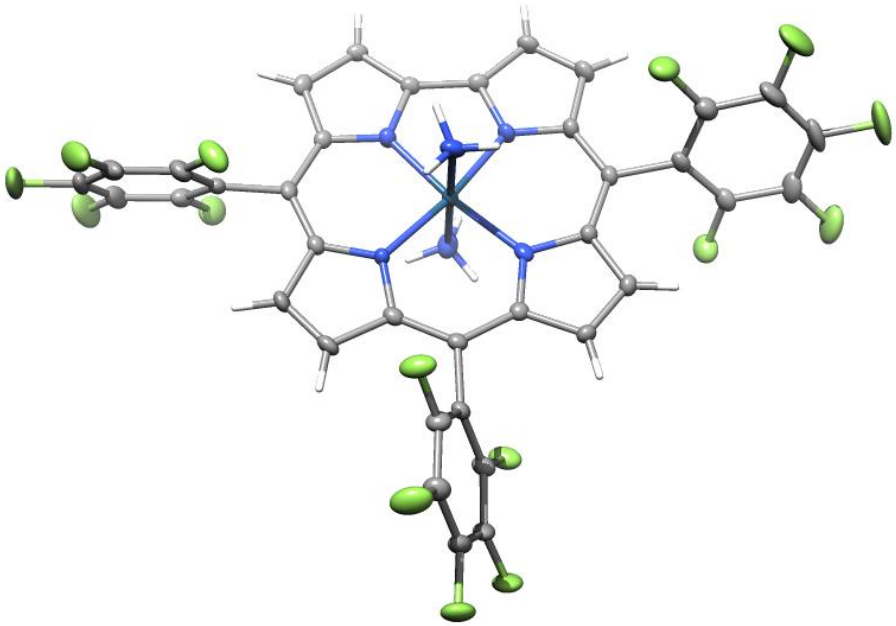

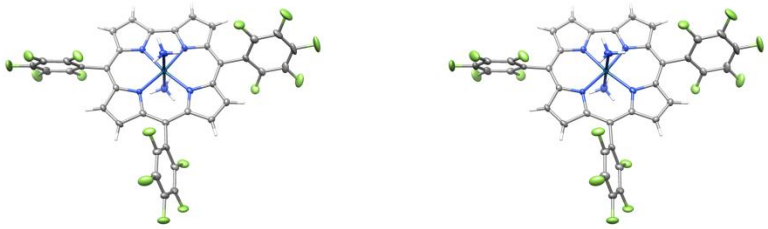

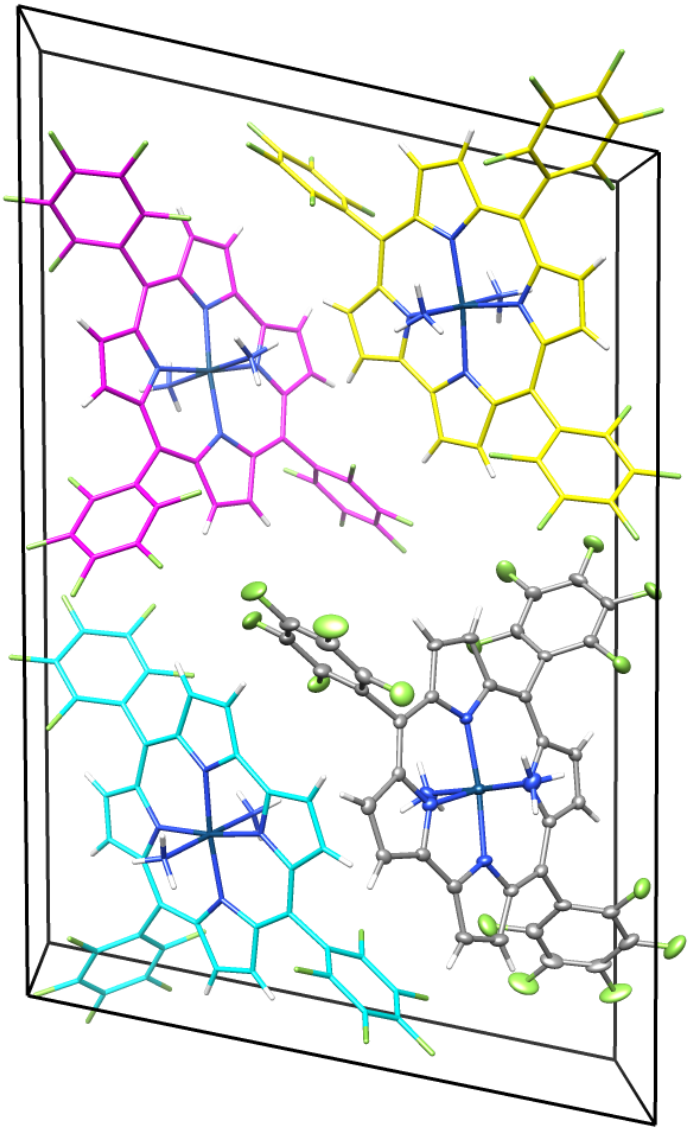

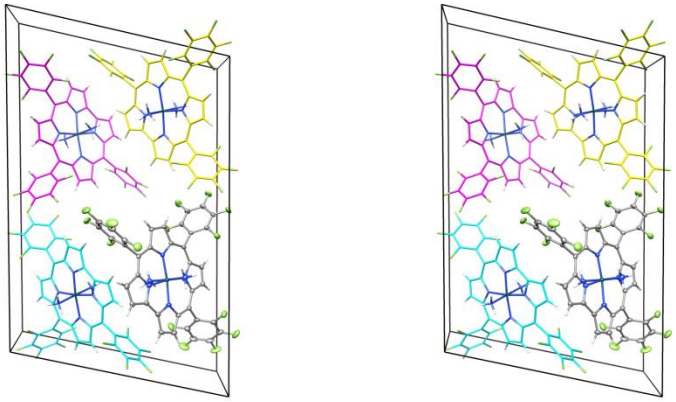

Table C-5-2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1-Ir(NH$_3$)$_2$** (CCDC 769388). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ir(1)	7129(1)	-800(1)	3129(1)	15(1)
F(1)	9824(1)	721(3)	2408(1)	34(1)
F(2)	10506(1)	2679(3)	1778(1)	46(1)
F(3)	9673(1)	4887(3)	1037(1)	55(1)
F(4)	8125(1)	5065(3)	923(1)	57(1)
F(5)	7441(1)	3191(3)	1565(1)	41(1)
F(6)	9513(1)	1159(3)	4684(1)	34(1)
F(7)	10160(1)	3191(3)	5512(1)	34(1)
F(8)	9346(1)	5923(3)	5869(1)	37(1)
F(9)	7906(1)	6778(3)	5356(1)	44(1)
F(10)	7280(1)	4880(3)	4502(1)	34(1)
F(11)	4617(1)	-467(3)	3853(1)	39(1)
F(12)	3571(1)	-1587(4)	4366(1)	59(1)
F(13)	3592(1)	-5235(4)	4719(1)	63(1)
F(14)	4696(1)	-7682(3)	4579(1)	57(1)
F(15)	5756(1)	-6561(3)	4065(1)	37(1)
N(1)	6295(1)	-2626(4)	2928(1)	17(1)
N(2)	7195(1)	-1293(3)	2429(1)	18(1)
N(3)	8000(1)	987(3)	3244(1)	17(1)
N(4)	6939(1)	-526(3)	3817(1)	15(1)
N(5)	6407(1)	1517(4)	2898(1)	24(1)

N(6)	7862(1)	-3038(4)	3382(1)	27(1)
C(1)	5798(2)	-3341(4)	3193(1)	15(1)
C(2)	5303(2)	-4625(4)	2860(1)	20(1)
C(3)	5534(2)	-4614(4)	2395(1)	18(1)
C(4)	6162(2)	-3341(4)	2442(1)	16(1)
C(5)	6678(2)	-2552(4)	2154(1)	18(1)
C(6)	6831(2)	-2561(5)	1659(1)	23(1)
C(7)	7425(2)	-1322(4)	1654(1)	24(1)
C(8)	7652(2)	-489(4)	2149(1)	18(1)
C(9)	8200(2)	895(4)	2363(1)	17(1)
C(10)	8370(2)	1583(4)	2873(1)	17(1)
C(11)	8926(2)	2956(4)	3098(1)	18(1)
C(12)	8880(2)	3177(4)	3594(1)	18(1)
C(13)	8281(2)	1948(4)	3683(1)	16(1)
C(14)	7983(2)	1740(4)	4126(1)	16(1)
C(15)	7364(2)	591(4)	4188(1)	17(1)
C(16)	7035(2)	352(4)	4631(1)	21(1)
C(17)	6436(2)	-864(4)	4506(1)	20(1)
C(18)	6366(2)	-1445(4)	3986(1)	16(1)
C(19)	5836(2)	-2731(4)	3701(1)	17(1)
C(20)	8608(2)	1881(4)	2008(1)	20(1)
C(21)	9390(2)	1793(4)	2048(1)	23(1)
C(22)	9754(2)	2800(5)	1725(1)	30(1)
C(23)	9324(2)	3903(5)	1350(1)	34(1)
C(24)	8548(2)	3994(5)	1292(1)	33(1)
C(25)	8201(2)	3007(5)	1619(1)	26(1)
C(26)	8365(2)	2897(4)	4576(1)	17(1)

C(27)	9102(2)	2537(5)	4841(1)	21(1)
C(28)	9437(2)	3563(5)	5271(1)	23(1)
C(29)	9030(2)	4955(5)	5443(1)	26(1)
C(30)	8301(2)	5399(5)	5188(1)	26(1)
C(31)	7984(2)	4378(5)	4755(1)	23(1)
C(32)	5228(2)	-3463(5)	3952(1)	18(1)
C(33)	4649(2)	-2275(5)	4030(1)	28(1)
C(34)	4104(2)	-2847(6)	4287(1)	36(1)
C(35)	4125(2)	-4654(6)	4465(1)	38(1)
C(36)	4676(2)	-5907(6)	4392(1)	35(1)
C(37)	5221(2)	-5311(5)	4132(1)	25(1)

Table C-5-3. Selected bond lengths [Å] and angles [°] for **1-Ir(NH$_3$)$_2$** (CCDC 769388)

Ir(1)-N(2)	1.957(2)	N(2)-Ir(1)-N(1)	79.51(9)
Ir(1)-N(1)	1.952(2)	N(2)-Ir(1)-N(4)	172.25(10)
Ir(1)-N(4)	1.975(2)	N(1)-Ir(1)-N(4)	92.77(9)
Ir(1)-N(3)	1.971(2)	N(2)-Ir(1)-N(3)	93.06(9)
Ir(1)-N(6)	2.064(3)	N(1)-Ir(1)-N(3)	172.55(9)
Ir(1)-N(5)	2.084(2)	N(4)-Ir(1)-N(3)	94.67(9)
		N(2)-Ir(1)-N(6)	91.16(10)
		N(1)-Ir(1)-N(6)	89.32(10)
		N(4)-Ir(1)-N(6)	89.29(10)
		N(3)-Ir(1)-N(6)	90.29(10)
		N(2)-Ir(1)-N(5)	90.56(10)
		N(1)-Ir(1)-N(5)	92.24(10)
		N(4)-Ir(1)-N(5)	89.18(9)
		N(3)-Ir(1)-N(5)	88.35(10)
		N(6)-Ir(1)-N(5)	177.86(10)

Table C-5-4. Bond lengths [Å] and angles [°] for **1-Ir(NH$_3$)$_2$** (CCDC 769388)

Ir(1)-N(2)	1.957(2)	N(3)-C(13)	1.363(3)
Ir(1)-N(1)	1.952(2)	N(3)-C(10)	1.384(3)
Ir(1)-N(4)	1.975(2)	N(4)-C(15)	1.368(3)
Ir(1)-N(3)	1.971(2)	N(4)-C(18)	1.371(3)
Ir(1)-N(6)	2.064(3)	C(1)-C(19)	1.429(4)
Ir(1)-N(5)	2.084(2)	C(1)-C(2)	1.435(4)
F(1)-C(21)	1.339(3)	C(2)-C(3)	1.408(4)
F(2)-C(22)	1.325(4)	C(3)-C(4)	1.419(4)
F(3)-C(23)	1.346(3)	C(4)-C(5)	1.444(4)
F(4)-C(24)	1.344(4)	C(5)-C(6)	1.426(4)
F(5)-C(25)	1.343(4)	C(6)-C(7)	1.375(4)
F(6)-C(27)	1.338(3)	C(7)-C(8)	1.437(4)
F(7)-C(28)	1.344(3)	C(8)-C(9)	1.411(4)
F(8)-C(29)	1.351(3)	C(9)-C(10)	1.430(4)
F(9)-C(30)	1.335(3)	C(9)-C(20)	1.498(4)
F(10)-C(31)	1.345(3)	C(10)-C(11)	1.423(4)
F(11)-C(33)	1.351(4)	C(11)-C(12)	1.370(4)
F(12)-C(34)	1.350(4)	C(12)-C(13)	1.437(4)
F(13)-C(35)	1.354(3)	C(13)-C(14)	1.423(4)
F(14)-C(36)	1.340(4)	C(14)-C(15)	1.409(4)
F(15)-C(37)	1.339(4)	C(14)-C(26)	1.498(4)
N(1)-C(1)	1.354(3)	C(15)-C(16)	1.456(4)
N(1)-C(4)	1.380(3)	C(16)-C(17)	1.355(4)
N(2)-C(8)	1.353(3)	C(17)-C(18)	1.446(4)
N(2)-C(5)	1.374(4)	C(18)-C(19)	1.410(4)

C(19)-C(32)	1.492(4)	N(1)-Ir(1)-N(6)	89.32(10)
C(20)-C(21)	1.382(4)	N(4)-Ir(1)-N(6)	89.29(10)
C(20)-C(25)	1.388(4)	N(3)-Ir(1)-N(6)	90.29(10)
C(21)-C(22)	1.390(4)	N(2)-Ir(1)-N(5)	90.56(10)
C(22)-C(23)	1.373(5)	N(1)-Ir(1)-N(5)	92.24(10)
C(23)-C(24)	1.365(5)	N(4)-Ir(1)-N(5)	89.18(9)
C(24)-C(25)	1.374(4)	N(3)-Ir(1)-N(5)	88.35(10)
C(26)-C(27)	1.383(4)	N(6)-Ir(1)-N(5)	177.86(10)
C(26)-C(31)	1.386(4)	C(1)-N(1)-C(4)	111.9(2)
C(27)-C(28)	1.388(4)	C(1)-N(1)-Ir(1)	130.24(18)
C(28)-C(29)	1.358(4)	C(4)-N(1)-Ir(1)	117.82(18)
C(29)-C(30)	1.375(4)	C(8)-N(2)-C(5)	112.4(2)
C(30)-C(31)	1.384(4)	C(8)-N(2)-Ir(1)	129.84(19)
C(32)-C(33)	1.381(4)	C(5)-N(2)-Ir(1)	117.58(18)
C(32)-C(37)	1.385(4)	C(13)-N(3)-C(10)	109.9(2)
C(33)-C(34)	1.376(4)	C(13)-N(3)-Ir(1)	125.55(18)
C(34)-C(35)	1.352(5)	C(10)-N(3)-Ir(1)	124.27(19)
C(35)-C(36)	1.366(5)	C(15)-N(4)-C(18)	111.2(2)
C(36)-C(37)	1.386(4)	C(15)-N(4)-Ir(1)	124.51(18)
		C(18)-N(4)-Ir(1)	124.32(18)
N(2)-Ir(1)-N(1)	79.51(9)	N(1)-C(1)-C(19)	120.0(2)
N(2)-Ir(1)-N(4)	172.25(10)	N(1)-C(1)-C(2)	106.6(2)
N(1)-Ir(1)-N(4)	92.77(9)	C(19)-C(1)-C(2)	133.4(3)
N(2)-Ir(1)-N(3)	93.06(9)	C(3)-C(2)-C(1)	107.3(3)
N(1)-Ir(1)-N(3)	172.55(9)	C(2)-C(3)-C(4)	107.7(3)
N(4)-Ir(1)-N(3)	94.67(9)	N(1)-C(4)-C(3)	106.4(2)
N(2)-Ir(1)-N(6)	91.16(10)	N(1)-C(4)-C(5)	112.3(2)

C(3)-C(4)-C(5)	141.3(3)	C(16)-C(17)-C(18)	108.5(2)
N(2)-C(5)-C(6)	105.6(3)	N(4)-C(18)-C(19)	125.5(2)
N(2)-C(5)-C(4)	112.8(2)	N(4)-C(18)-C(17)	106.3(2)
C(6)-C(5)-C(4)	141.6(3)	C(19)-C(18)-C(17)	128.2(3)
C(7)-C(6)-C(5)	108.2(3)	C(18)-C(19)-C(1)	127.1(2)
C(6)-C(7)-C(8)	108.1(2)	C(18)-C(19)-C(32)	116.2(2)
N(2)-C(8)-C(9)	120.4(2)	C(1)-C(19)-C(32)	116.6(2)
N(2)-C(8)-C(7)	105.7(2)	C(21)-C(20)-C(25)	116.2(3)
C(9)-C(8)-C(7)	133.9(3)	C(21)-C(20)-C(9)	123.8(3)
C(8)-C(9)-C(10)	127.7(2)	C(25)-C(20)-C(9)	120.0(3)
C(8)-C(9)-C(20)	116.4(2)	F(1)-C(21)-C(20)	120.0(3)
C(10)-C(9)-C(20)	115.7(2)	F(1)-C(21)-C(22)	117.7(3)
N(3)-C(10)-C(9)	124.4(3)	C(20)-C(21)-C(22)	122.3(3)
N(3)-C(10)-C(11)	106.9(2)	F(2)-C(22)-C(23)	120.6(3)
C(9)-C(10)-C(11)	128.7(2)	F(2)-C(22)-C(21)	120.3(3)
C(12)-C(11)-C(10)	108.2(2)	C(23)-C(22)-C(21)	119.1(3)
C(11)-C(12)-C(13)	107.5(3)	F(3)-C(23)-C(24)	120.3(3)
N(3)-C(13)-C(14)	123.3(3)	F(3)-C(23)-C(22)	119.4(3)
N(3)-C(13)-C(12)	107.3(2)	C(24)-C(23)-C(22)	120.3(3)
C(14)-C(13)-C(12)	129.3(3)	F(4)-C(24)-C(23)	120.5(3)
C(15)-C(14)-C(13)	127.4(3)	F(4)-C(24)-C(25)	119.9(3)
C(15)-C(14)-C(26)	116.4(2)	C(23)-C(24)-C(25)	119.6(3)
C(13)-C(14)-C(26)	116.2(2)	F(5)-C(25)-C(24)	118.1(3)
N(4)-C(15)-C(14)	124.5(2)	F(5)-C(25)-C(20)	119.3(3)
N(4)-C(15)-C(16)	106.3(2)	C(24)-C(25)-C(20)	122.6(3)
C(14)-C(15)-C(16)	129.3(3)	C(27)-C(26)-C(31)	116.1(3)
C(17)-C(16)-C(15)	107.8(3)	C(27)-C(26)-C(14)	122.7(3)

C(31)-C(26)-C(14)	121.1(3)	C(34)-C(35)-C(36)	121.0(3)
F(6)-C(27)-C(28)	118.2(3)	F(14)-C(36)-C(35)	120.1(3)
F(6)-C(27)-C(26)	119.6(3)	F(14)-C(36)-C(37)	120.5(4)
C(28)-C(27)-C(26)	122.1(3)	C(35)-C(36)-C(37)	119.4(3)
F(7)-C(28)-C(29)	120.3(3)	F(15)-C(37)-C(36)	118.4(3)
F(7)-C(28)-C(27)	120.2(3)	F(15)-C(37)-C(32)	120.1(3)
C(29)-C(28)-C(27)	119.6(3)	C(36)-C(37)-C(32)	121.5(3)
F(8)-C(29)-C(30)	119.5(3)		
F(8)-C(29)-C(28)	119.9(3)		
C(30)-C(29)-C(28)	120.7(3)		
F(9)-C(30)-C(29)	120.5(3)		
F(9)-C(30)-C(31)	120.8(3)		
C(29)-C(30)-C(31)	118.7(3)		
F(10)-C(31)-C(30)	117.6(3)		
F(10)-C(31)-C(26)	119.6(3)		
C(30)-C(31)-C(26)	122.7(3)		
C(33)-C(32)-C(37)	116.3(3)		
C(33)-C(32)-C(19)	120.6(3)		
C(37)-C(32)-C(19)	123.0(3)		
F(11)-C(33)-C(34)	118.2(3)		
F(11)-C(33)-C(32)	119.0(3)		
C(34)-C(33)-C(32)	122.8(3)		
F(12)-C(34)-C(35)	121.4(3)		
F(12)-C(34)-C(33)	119.6(4)		
C(35)-C(34)-C(33)	119.0(3)		
F(13)-C(35)-C(34)	119.7(4)		
F(13)-C(35)-C(36)	119.4(4)		

Table C-5-5. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for **1-Ir(NH$_3$)$_2$** (CCDC 769388). The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$.

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ir(1)	164(1)	178(1)	115(1)	-11(1)	46(1)	-16(1)
F(1)	265(10)	384(12)	379(10)	59(9)	119(9)	85(10)
F(2)	406(13)	455(14)	646(14)	-104(12)	360(11)	-85(12)
F(3)	920(19)	400(13)	470(13)	13(11)	487(13)	-197(14)
F(4)	861(18)	477(14)	312(11)	219(10)	18(12)	-52(14)
F(5)	352(12)	445(14)	367(11)	131(9)	-42(10)	15(11)
F(6)	312(11)	421(13)	252(9)	-36(8)	-4(9)	133(10)
F(7)	257(10)	482(13)	230(9)	-5(9)	-70(8)	-5(10)
F(8)	372(12)	436(13)	242(9)	-140(9)	-41(9)	-74(11)
F(9)	391(12)	429(14)	444(12)	-244(10)	-15(10)	54(11)
F(10)	252(10)	380(11)	331(10)	-129(9)	-42(9)	92(10)
F(11)	433(13)	476(14)	302(10)	98(9)	165(10)	227(11)
F(12)	311(12)	1190(20)	307(11)	-32(12)	157(10)	186(14)
F(13)	486(14)	1130(20)	336(12)	-57(13)	241(11)	-416(15)
F(14)	845(18)	471(15)	423(13)	62(11)	215(12)	-360(14)
F(15)	433(13)	252(11)	433(12)	84(9)	92(10)	4(10)
N(1)	191(13)	169(13)	166(11)	-7(10)	65(10)	-14(11)
N(2)	211(13)	220(14)	137(11)	-19(9)	72(10)	-22(11)
N(3)	174(12)	206(14)	136(10)	37(10)	39(9)	60(11)
N(4)	139(12)	185(14)	122(10)	-9(9)	44(9)	-23(10)

N(5)	267(15)	257(14)	155(12)	-6(10)	-17(11)	-20(13)
N(6)	245(15)	263(16)	323(15)	-20(11)	122(12)	-8(13)
C(1)	152(15)	133(14)	176(13)	7(11)	37(11)	17(12)
C(2)	184(15)	164(17)	247(15)	32(11)	57(13)	9(12)
C(3)	192(15)	145(16)	176(13)	-19(10)	6(12)	11(12)
C(4)	193(15)	149(15)	149(13)	-15(11)	29(12)	15(13)
C(5)	195(15)	168(15)	177(13)	-34(11)	28(12)	6(14)
C(6)	268(17)	263(17)	144(13)	-32(12)	30(12)	-26(15)
C(7)	291(18)	285(18)	154(14)	-6(12)	86(13)	-20(15)
C(8)	198(15)	213(18)	157(13)	0(11)	70(12)	-33(13)
C(9)	180(15)	183(15)	169(12)	21(12)	67(11)	0(14)
C(10)	174(15)	180(15)	159(13)	6(11)	46(12)	-22(13)
C(11)	166(15)	167(16)	202(14)	11(11)	60(12)	-14(12)
C(12)	159(15)	181(16)	176(14)	-15(11)	20(12)	-35(13)
C(13)	152(14)	153(15)	164(13)	12(10)	26(11)	18(12)
C(14)	171(15)	169(15)	134(13)	1(10)	17(11)	19(13)
C(15)	188(15)	192(16)	139(12)	12(11)	32(11)	38(13)
C(16)	259(17)	257(18)	110(12)	1(11)	55(12)	27(14)
C(17)	217(15)	246(16)	139(12)	34(12)	79(11)	-9(15)
C(18)	175(15)	177(15)	151(13)	23(11)	53(12)	18(13)
C(19)	158(14)	192(16)	171(13)	58(11)	50(11)	24(13)
C(20)	275(18)	197(17)	132(13)	-18(11)	69(12)	-43(14)
C(21)	296(18)	232(18)	181(14)	-6(12)	98(13)	-3(15)
C(22)	360(20)	271(19)	342(18)	-69(15)	234(16)	-57(17)
C(23)	600(30)	240(20)	249(16)	0(13)	258(18)	-108(18)
C(24)	520(20)	280(20)	184(15)	86(14)	50(16)	-12(19)
C(25)	304(19)	260(19)	225(15)	22(13)	47(14)	-11(16)

C(26)	199(16)	201(16)	120(13)	5(11)	38(12)	-18(13)
C(27)	230(16)	233(16)	157(13)	-3(12)	33(12)	38(15)
C(28)	190(16)	318(18)	150(14)	36(12)	-15(12)	-29(15)
C(29)	297(19)	288(17)	164(14)	-22(13)	6(13)	-114(16)
C(30)	294(19)	251(19)	223(15)	-69(12)	50(14)	5(15)
C(31)	187(16)	264(18)	207(14)	-7(13)	-4(12)	20(15)
C(32)	165(15)	263(16)	120(13)	3(11)	17(11)	-34(14)
C(33)	282(18)	400(20)	163(14)	49(14)	54(13)	18(17)
C(34)	209(18)	720(30)	154(15)	-28(17)	47(14)	50(20)
C(35)	300(20)	700(30)	162(15)	-29(16)	92(15)	-250(20)
C(36)	420(20)	410(20)	210(15)	36(16)	50(15)	-210(20)
C(37)	242(17)	290(20)	203(15)	22(12)	-1(13)	-51(15)