Supporting information available

Aminolysis of iridium thiophene compounds

M. Angeles Paz-Sandoval,* Marisol Cervantes-Vásquez, and Brenda A. Paz-Michel

Departamento de Química, Cinvestav,
Av. IPN # 2508 esq. Ticomán, San Pedro Zacatenco, México 07360, D.F. México
E-mail: mpaz@cinvestav.mx

Dedicated to Professor Rosalinda Contreras, friend and colleague, on the ocassion of her 60th birthday in recognition of her oustanding contribution to the main group chemistry

Supporting information for crystal structures of compounds:

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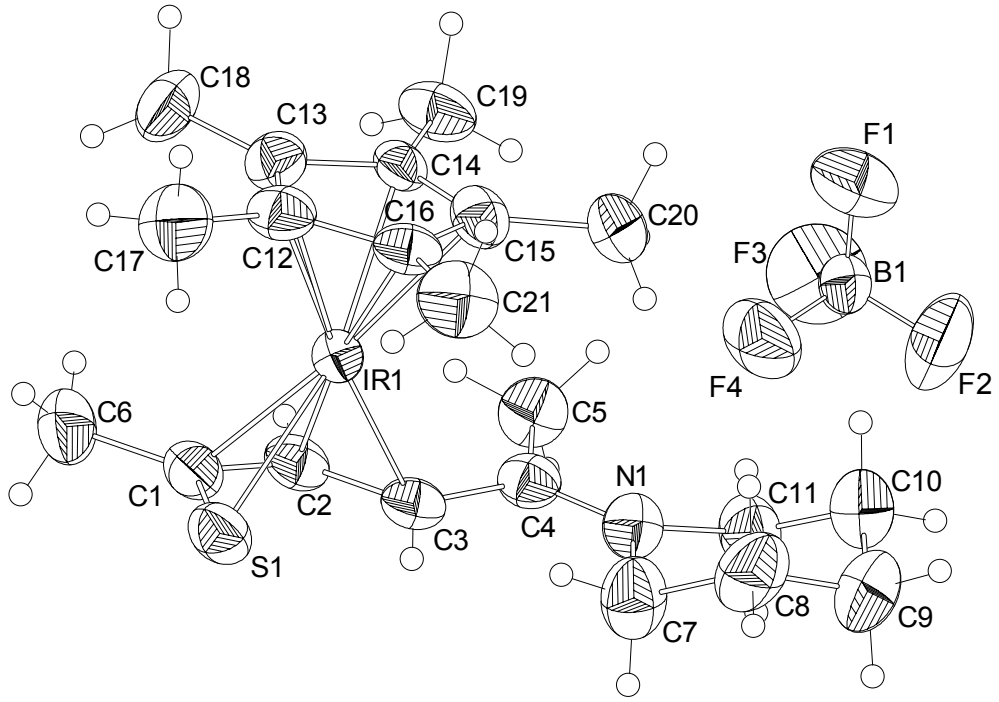

ORTEP drawing of Compound **12**

Formula: C_{21} H_{33} B F_4 Ir N S

Authors : Marisol Cervantes Vásquez y Ma. de los Ángeles Paz Sandoval.

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Table 1. Crystal data and data collection

Identification code	Compound **12**	
Operator	MLR and BPM	
Empirical formula	C_{21} H_{33} B F_4 Ir N S	
Formula weight	610.55	
Crystal size	0.56 x 0.45 x 0.33 mm	
Crystal color and habit	red prism	
Crystal system	Monoclinic	
Space group	P2/c	
Unit cell dimensions	a = 13.450(3) Å	α = 90.00(2)°
	b = 7.877(3) Å	β = 91.34(2)°
	c = 21.840(3) Å	γ = 90.00(2)°
Volume	2313.2(11) $Å^3$	
Z	4	
Density (calculated)	1.753 Mg/m^3	
Absorption coefficient	5.901 mm^{-1}	
F(000)	1200	
Diffractometer used	Enraf-Nonius CAD4	
Radiation and wavelength	MoKα with λ=0.71073 Å	
Scan type	ω/2θ	
Temperature	270(2) K	
2θ range for data collection	5.18 to 51.92°	
Index ranges	$-16 \le h \le 16$ $0 \le k \le 9$ $0 \le l \le 26$	
Reflections collected	4527	
Independent reflections	4527 (R_{int} = 0.0000)	
Observed reflections	3635 (F>4σ(F))	
Absorption correction	Semi-empirical	
Max. and min. transmission	0.2462 and 0.1367	

Experimental details :

Scan speed	Variable; 16.1 to 60 °/min in ω
Scan range (ω)	0.7 °

Background measurement : Moving crystal and moving counter at the beginning and end of scan, each for 25% of total scan area.

Crystal mounted in perfluorpolyether oil

Table 2. Solution and refinement

Structure solution program	SHELXS-97(Sheldrick 1990)
Solution	heavy-atom-method
Refinement method	Full-matrix Least-Squares on F^2
Hydrogen atoms	mixed
Weighting scheme	$w^{-1}=\sigma^2Fo^2+(P)^2+P$ where $P=(Fo^2+2Fc^2)/3$
Data / restraints / parameters	4527 / 0 / 277
Data-to-parameter-ratio	16.3 : 1 (13.1 : 1 [F>4σ(F)])
Final R indices [F>4σ(F)]	R1 = 0.0282, wR2 = 0.0801
R indices (all data)	R1 = 0.0416, wR2 = 0.0846
Goodness-of-Fit on F^2	1.081
Largest and mean Δ/σ	0.012 0.002
Largest difference peak	0.888 eÅ^{-3}
Largest difference hole	-1.013 eÅ^{-3}

Refinement details :

Program used	SHELXL-97 (Sheldrick 1997)
CifRtf version used	2.0

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **12**. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U(eq)
C(1)	1666(4)	-174(6)	3618(2)	46.6(12)
C(2)	1364(3)	385(6)	4202(2)	43.1(11)
C(3)	2099(4)	461(6)	4681(2)	42.6(11)
C(4)	1956(3)	1284(6)	5260(2)	41.8(10)
C(5)	991(4)	2112(7)	5393(3)	55.7(14)
C(6)	956(4)	-259(8)	3079(3)	64.5(15)
C(7)	3627(4)	398(9)	5586(3)	65.9(16)
C(8)	4484(4)	1350(10)	5912(3)	72.7(17)
C(9)	4285(6)	1628(10)	6584(3)	85(2)
C(10)	3334(6)	2589(9)	6638(4)	75.8(19)
C(11)	2462(5)	1696(8)	6342(3)	63.1(16)
C(12)	3108(4)	3675(6)	3197(2)	47.4(12)
C(13)	2124(4)	4241(6)	3319(2)	46.4(11)
C(14)	2117(3)	4763(5)	3957(2)	36.9(10)
C(15)	3086(4)	4547(6)	4211(2)	45.0(11)
C(16)	3699(3)	3844(5)	3751(2)	43.8(11)
C(17)	3468(5)	3083(7)	2590(3)	69.3(18)
C(18)	1271(5)	4378(8)	2885(3)	68.6(16)
C(19)	1240(4)	5565(6)	4264(3)	57.4(14)
C(20)	3412(4)	5074(7)	4843(3)	59.5(14)
C(21)	4797(4)	3516(8)	3820(3)	68.1(16)
B(1)	8540(6)	2888(8)	3870(3)	53.2(15)
F(1)	8833(4)	4474(5)	3712(2)	112.9(16)
F(2)	8994(5)	2349(7)	4390(2)	126(2)
F(3)	7528(3)	2908(9)	3944(2)	127(3)
F(4)	8723(4)	1791(6)	3412(2)	105.0(16)
Ir(1)	2515.8(1)	2043.3(2)	3907.7(1)	33.9(1)
N(1)	2652(3)	1239(6)	5691.3(19)	48.8(10)
S(1)	2913.2(10)	-765.5(16)	3555.4(6)	50.2(3)

Table 4. Bond lengths [Å] and angles [°] for compound **12**

C(1)-C(2)	1.417(7)	C(1)-C(6)	1.500(7)
C(1)-S(1)	1.750(5)	C(1)-Ir(1)	2.173(5)
C(2)-C(3)	1.423(7)	C(2)-Ir(1)	2.137(4)
C(2)-H(2)	0.95(4)	C(3)-C(4)	1.438(7)
C(3)-Ir(1)	2.182(5)	C(3)-H(3)	0.67(4)
C(4)-N(1)	1.313(6)	C(4)-C(5)	1.488(7)
C(7)-N(1)	1.491(6)	C(7)-C(8)	1.537(8)
C(8)-C(9)	1.514(9)	C(9)-C(10)	1.493(11)
C(10)-C(11)	1.501(9)	C(11)-N(1)	1.494(7)
C(12)-C(13)	1.428(7)	C(12)-C(16)	1.439(7)
C(12)-C(17)	1.497(7)	C(12)-Ir(1)	2.179(5)
C(13)-C(14)	1.452(7)	C(13)-C(18)	1.476(7)
C(13)-Ir(1)	2.212(5)	C(14)-C(15)	1.415(7)
C(14)-C(19)	1.509(6)	C(14)-Ir(1)	2.212(4)
C(15)-C(16)	1.426(6)	C(15)-C(20)	1.499(7)
C(15)-Ir(1)	2.211(5)	C(16)-C(21)	1.503(7)
C(16)-Ir(1)	2.165(4)	Ir(1)-S(1)	2.4066(15)
B(1)-F(2)	1.345(8)	B(1)-F(4)	1.349(8)
B(1)-F(1)	1.358(8)	B(1)-F(3)	1.374(8)
C(2)-C(1)-C(6)	122.0(5)	C(2)-C(1)-S(1)	116.7(4)
C(6)-C(1)-S(1)	121.3(4)	C(2)-C(1)-Ir(1)	69.4(3)
C(6)-C(1)-Ir(1)	125.8(4)	S(1)-C(1)-Ir(1)	74.80(18)
C(1)-C(2)-C(3)	117.7(4)	C(1)-C(2)-Ir(1)	72.2(3)
C(3)-C(2)-Ir(1)	72.5(3)	C(1)-C(2)-H(2)	117(3)
C(3)-C(2)-H(2)	125(3)	Ir(1)-C(2)-H(2)	116(3)
C(2)-C(3)-C(4)	124.0(5)	C(2)-C(3)-Ir(1)	69.1(3)
C(4)-C(3)-Ir(1)	117.7(3)	C(2)-C(3)-H(3)	115(4)
C(4)-C(3)-H(3)	111(4)	Ir(1)-C(3)-H(3)	115(4)
N(1)-C(4)-C(3)	120.8(4)	N(1)-C(4)-C(5)	118.8(5)
C(3)-C(4)-C(5)	120.3(5)	C(4)-C(5)-H(5A)	109.5
N(1)-C(7)-C(8)	111.3(5)	C(9)-C(8)-C(7)	111.8(6)
C(10)-C(9)-C(8)	108.8(6)	C(11)-C(10)-C(9)	113.0(6)
N(1)-C(11)-C(10)	111.9(6)	C(13)-C(12)-C(16)	108.1(4)
C(13)-C(12)-C(17)	125.7(5)	C(16)-C(12)-C(17)	126.1(5)
C(13)-C(12)-Ir(1)	72.3(3)	C(16)-C(12)-Ir(1)	70.1(3)
C(17)-C(12)-Ir(1)	125.3(4)	C(12)-C(13)-C(14)	107.1(4)
C(12)-C(13)-C(18)	127.8(5)	C(14)-C(13)-C(18)	125.0(5)
C(12)-C(13)-Ir(1)	69.8(3)	C(14)-C(13)-Ir(1)	70.8(3)
C(18)-C(13)-Ir(1)	127.0(4)	C(15)-C(14)-C(13)	108.4(4)

C(15)-C(14)-C(19)	126.8(4)	C(13)-C(14)-C(19)	124.6(5)
C(15)-C(14)-Ir(1)	71.3(3)	C(13)-C(14)-Ir(1)	70.9(3)
C(19)-C(14)-Ir(1)	128.4(3)	C(14)-C(15)-C(16)	108.3(4)
C(14)-C(15)-C(20)	125.1(5)	C(16)-C(15)-C(20)	126.5(5)
C(14)-C(15)-Ir(1)	71.4(2)	C(16)-C(15)-Ir(1)	69.2(3)
C(20)-C(15)-Ir(1)	128.0(4)	C(15)-C(16)-C(12)	108.0(4)
C(15)-C(16)-C(21)	125.4(5)	C(12)-C(16)-C(21)	126.2(5)
C(15)-C(16)-Ir(1)	72.8(3)	C(12)-C(16)-Ir(1)	71.2(3)
C(21)-C(16)-Ir(1)	126.6(3)	F(2)-B(1)-F(4)	109.7(6)
F(2)-B(1)-F(1)	112.1(6)	F(4)-B(1)-F(1)	110.0(6)
F(2)-B(1)-F(3)	109.7(6)	F(4)-B(1)-F(3)	107.0(6)
F(1)-B(1)-F(3)	108.3(6)	C(2)-Ir(1)-C(16)	171.38(19)
C(2)-Ir(1)-C(1)	38.39(19)	C(16)-Ir(1)-C(1)	149.83(19)
C(2)-Ir(1)-C(12)	148.7(2)	C(16)-Ir(1)-C(12)	38.69(19)
C(1)-Ir(1)-C(12)	117.7(2)	C(2)-Ir(1)-C(3)	38.44(19)
C(16)-Ir(1)-C(3)	134.37(19)	C(1)-Ir(1)-C(3)	67.84(19)
C(12)-Ir(1)-C(3)	172.8(2)	C(2)-Ir(1)-C(13)	119.23(19)
C(16)-Ir(1)-C(13)	64.03(18)	C(1)-Ir(1)-C(13)	110.1(2)
C(12)-Ir(1)-C(13)	37.93(18)	C(3)-Ir(1)-C(13)	146.53(19)
C(2)-Ir(1)-C(14)	113.50(17)	C(16)-Ir(1)-C(14)	63.47(17)
C(1)-Ir(1)-C(14)	131.74(17)	C(12)-Ir(1)-C(14)	63.68(17)
C(3)-Ir(1)-C(14)	116.66(18)	C(13)-Ir(1)-C(14)	38.32(18)
C(2)-Ir(1)-C(15)	134.70(18)	C(16)-Ir(1)-C(15)	38.00(17)
C(1)-Ir(1)-C(15)	168.50(18)	C(12)-Ir(1)-C(15)	63.73(19)
C(3)-Ir(1)-C(15)	111.80(19)	C(13)-Ir(1)-C(15)	63.4(2)
C(14)-Ir(1)-C(15)	37.31(18)	C(2)-Ir(1)-S(1)	72.69(14)
C(16)-Ir(1)-S(1)	112.48(13)	C(1)-Ir(1)-S(1)	44.57(13)
C(12)-Ir(1)-S(1)	103.13(13)	C(3)-Ir(1)-S(1)	77.59(15)
C(13)-Ir(1)-S(1)	125.84(14)	C(14)-Ir(1)-S(1)	164.15(13)
C(15)-Ir(1)-S(1)	146.87(13)	C(4)-N(1)-C(7)	121.0(4)
C(4)-N(1)-C(11)	122.8(5)	C(7)-N(1)-C(11)	115.2(5)
C(1)-S(1)-Ir(1)	60.63(16)		

Table 5. Anisotropic displacement parameters [$Å^2 \times 10^3$]

	U11	U22	U33	U23	U13	U12
C(1)	48(3)	37(2)	54(3)	-6(2)	-5(2)	0(2)
C(2)	37(2)	34(2)	58(3)	0(2)	3(2)	-8.6(19)
C(3)	44(3)	31(2)	53(3)	4(2)	4(2)	-4(2)
C(4)	44(2)	37(2)	45(3)	4(2)	9(2)	-3(2)
C(5)	47(3)	62(3)	58(4)	-1(3)	4(3)	5(2)
C(6)	66(4)	65(3)	62(4)	-12(3)	-18(3)	-5(3)
C(7)	50(3)	83(4)	64(4)	-13(3)	-7(3)	8(3)
C(8)	55(3)	90(4)	72(4)	5(4)	-16(3)	13(3)
C(9)	95(5)	92(5)	67(5)	0(4)	-34(4)	7(4)
C(10)	92(6)	73(4)	62(4)	-8(4)	-17(4)	-6(4)
C(11)	79(4)	64(3)	47(3)	-8(3)	5(3)	-10(3)
C(12)	53(3)	38(2)	51(3)	8(2)	11(2)	-3(2)
C(13)	50(3)	46(3)	43(3)	6(2)	1(2)	-1(2)
C(14)	49(2)	26.5(19)	36(2)	-1.2(18)	5(2)	-7.9(19)
C(15)	46(3)	42(2)	47(3)	-3(2)	5(2)	-13(2)
C(16)	43(2)	31(2)	58(3)	7(2)	7(2)	-5(2)
C(17)	86(5)	75(4)	47(4)	-2(3)	20(3)	10(3)
C(18)	80(4)	76(4)	49(3)	4(3)	-20(3)	18(3)
C(19)	64(3)	40(3)	69(4)	-5(3)	17(3)	11(2)
C(20)	68(3)	50(3)	60(3)	-8(3)	-11(3)	-13(3)
C(21)	41(3)	70(3)	92(5)	3(4)	1(3)	-11(3)
B(1)	61(4)	57(4)	42(3)	-4(3)	0(3)	1(3)
F(1)	142(4)	67(2)	129(4)	-6(3)	-2(3)	-19(3)
F(2)	145(5)	163(5)	69(3)	17(3)	-31(3)	13(4)
F(3)	73(4)	159(8)	151(7)	-5(3)	30(4)	7(3)
F(4)	149(5)	89(3)	78(3)	-25(2)	30(3)	-2(3)
Ir(1)	33.8(1)	34.0(1)	33.9(1)	-1.5(1)	0.9(1)	-1.3(1)
N(1)	48(2)	53(2)	46(2)	-1(2)	1.3(18)	-2(2)
S(1)	52.8(7)	41.3(6)	56.4(8)	-10.6(6)	2.0(6)	6.5(5)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for compound **12**

	x	y	z	U(eq)
H(5A)	628	1417	5671	84
H(5B)	610	2248	5019	84
H(5C)	1112	3205	5574	84
H(6A)	671	-1374	3053	97
H(6B)	1307	-19	2711	97
H(6C)	437	563	3128	97
H(7A)	3745	359	5149	79
H(7B)	3605	-761	5736	79
H(8A)	5093	705	5873	87
H(8B)	4577	2441	5715	87
H(9A)	4236	543	6791	102
H(9B)	4827	2264	6773	102
H(10A)	3202	2763	7068	91
H(10B)	3408	3696	6450	91
H(11A)	2320	672	6571	76
H(11B)	1882	2426	6356	76
H(17A)	2909	2777	2332	104
H(17B)	3892	2114	2649	104
H(17C)	3833	3979	2400	104
H(18A)	1212	5528	2743	103
H(18B)	672	4056	3086	103
H(18C)	1373	3639	2542	103
H(19A)	1303	5407	4699	86
H(19B)	636	5042	4115	86
H(19C)	1222	6757	4173	86
H(20A)	3659	6217	4833	89
H(20B)	3929	4328	4991	89
H(20C)	2857	5015	5111	89
H(21A)	5155	4548	3748	102
H(21B)	4990	2672	3529	102
H(21C)	4947	3118	4228	102
H(2)	720(03)	880(06)	4220(02)	40(12)
H(3)	2370(03)	-240(06)	4720(02)	28(14)

Table 7. Crystal data and data collection parameters

Compound	Compound **12**
Chem. formula	C_{21} H_{33} B F_4 Ir N S
Form. wght.	610.55
Cryst. size [mm]	0.33x0.45x0.56
Cryst. system	Monoclinic
Space group	P2/c
a, [Å]	13.450(3)
b, [Å]	7.877(3)
c, [Å]	21.840(3)
α, [°]	90.00(2)
β, [°]	91.34(2)
γ, [°]	90.00(2)
V, [Å^3]	2313.2(11)
Z	4
ρ(calcd.), [Mg/m^3]	1.753
μ [mm^{-1}]	5.901
F(000)	1200
Index range	-16≤h≤160≤k≤90≤l≤26
2 θ [°]	51.92
Temp, [K]	270(2)
Refl. collected	4527
Refl. unique	4527
Refl. observed (4σ)	3635
R (int.)	0.0000
No. variables	277
Weighting scheme[1] x/y	/
GOOF	1.081
Final R (4σ)	0.0282
Final wR2	0.0801
Larg. res. peak [e/Å^3]	0.888

[1] $w^{-1} = \sigma^2 F_o^2 + (xP)^2 + yP$; $P = (F_o^2 + 2F_c^2)/3$

Selected torsion angles for compound 12

-178.41 (0.46) C6 - C1 - C2 - C3
1.56 (0.58) S1 - C1 - C2 - C3
-58.31 (0.38) Ir1 - C1 - C2 - C3
-120.10 (0.48) C6 - C1 - C2 - Ir1
59.87 (0.28) S1 - C1 - C2 - Ir1
168.15 (0.43) C1 - C2 - C3 - C4
109.99 (0.46) Ir1 - C2 - C3 - C4
58.16 (0.38) C1 - C2 - C3 - Ir1
176.89 (0.45) C2 - C3 - C4 - N1
-100.74 (0.50) Ir1 - C3 - C4 - N1
0.67 (0.72) C2 - C3 - C4 - C5
83.04 (0.50) Ir1 - C3 - C4 - C5
52.56 (0.75) N1 - C7 - C8 - C9
-57.67 (0.85) C7 - C8 - C9 - C10
58.37 (0.90) C8 - C9 - C10 - C11
-53.32 (0.83) C9 - C10 - C11 - N1
0.03 (0.51) C16 - C12 - C13 - C14
-177.49 (0.46) C17 - C12 - C13 - C14
61.33 (0.31) Ir1 - C12 - C13 - C14
176.95 (0.52) C16 - C12 - C13 - C18
-0.57 (0.85) C17 - C12 - C13 - C18
-121.75 (0.57) Ir1 - C12 - C13 - C18
-61.30 (0.31) C16 - C12 - C13 - Ir1
121.18 (0.50) C17 - C12 - C13 - Ir1
1.16 (0.52) C12 - C13 - C14 - C15
-175.87 (0.50) C18 - C13 - C14 - C15
61.82 (0.31) Ir1 - C13 - C14 - C15
175.39 (0.42) C12 - C13 - C14 - C19
-1.64 (0.77) C18 - C13 - C14 - C19
-123.95 (0.43) Ir1 - C13 - C14 - C19
-60.66 (0.32) C12 - C13 - C14 - Ir1
122.31 (0.53) C18 - C13 - C14 - Ir1
-1.91 (0.52) C13 - C14 - C15 - C16
-175.97 (0.42) C19 - C14 - C15 - C16
59.61 (0.32) Ir1 - C14 - C15 - C16
174.66 (0.44) C13 - C14 - C15 - C20
0.60 (0.74) C19 - C14 - C15 - C20

-123.81 (0.48) Ir1 - C14 - C15 - C20
-61.52 (0.31) C13 - C14 - C15 - Ir1
124.42 (0.45) C19 - C14 - C15 - Ir1
1.92 (0.51) C14 - C15 - C16 - C12
-174.59 (0.46) C20 - C15 - C16 - C12
62.87 (0.32) Ir1 - C15 - C16 - C12
176.04 (0.44) C14 - C15 - C16 - C21
-0.47 (0.79) C20 - C15 - C16 - C21
-123.01 (0.48) Ir1 - C15 - C16 - C21
-60.95 (0.31) C14 - C15 - C16 - Ir1
122.53 (0.50) C20 - C15 - C16 - Ir1
-1.19 (0.52) C13 - C12 - C16 - C15
176.31 (0.47) C17 - C12 - C16 - C15
-63.89 (0.32) Ir1 - C12 - C16 - C15
-175.25 (0.45) C13 - C12 - C16 - C21
2.25 (0.79) C17 - C12 - C16 - C21
122.05 (0.48) Ir1 - C12 - C16 - C21
62.69 (0.32) C13 - C12 - C16 - Ir1
-119.80 (0.50) C17 - C12 - C16 - Ir1
-164.08 (1.06) C1 - C2 - Ir1 - C16
-36.26 (1.25) C3 - C2 - Ir1 - C16
127.82 (0.43) C3 - C2 - Ir1 - C1
50.80 (0.48) C1 - C2 - Ir1 - C12
178.62 (0.33) C3 - C2 - Ir1 - C12
-127.82 (0.43) C1 - C2 - Ir1 - C3
85.82 (0.33) C1 - C2 - Ir1 - C13
-146.36 (0.30) C3 - C2 - Ir1 - C13
128.34 (0.28) C1 - C2 - Ir1 - C14
-103.84 (0.31) C3 - C2 - Ir1 - C14
166.16 (0.29) C1 - C2 - Ir1 - C15
-66.03 (0.39) C3 - C2 - Ir1 - C15
-36.07 (0.26) C1 - C2 - Ir1 - S1
91.75 (0.29) C3 - C2 - Ir1 - S1
-34.96 (1.25) C15 - C16 - Ir1 - C2
-151.59 (1.08) C12 - C16 - Ir1 - C2
86.76 (1.23) C21 - C16 - Ir1 - C2
164.84 (0.35) C15 - C16 - Ir1 - C1
48.22 (0.50) C12 - C16 - Ir1 - C1
-73.43 (0.66) C21 - C16 - Ir1 - C1
116.63 (0.42) C15 - C16 - Ir1 - C12

-121.65 (0.59) C21 - C16 - Ir1 - C12
-65.92 (0.39) C15 - C16 - Ir1 - C3
177.45 (0.28) C12 - C16 - Ir1 - C3
55.80 (0.57) C21 - C16 - Ir1 - C3
79.32 (0.32) C15 - C16 - Ir1 - C13
-37.31 (0.27) C12 - C16 - Ir1 - C13
-158.96 (0.54) C21 - C16 - Ir1 - C13
36.39 (0.28) C15 - C16 - Ir1 - C14
-80.24 (0.29) C12 - C16 - Ir1 - C14
158.11 (0.55) C21 - C16 - Ir1 - C14
-116.63 (0.42) C12 - C16 - Ir1 - C15
121.72 (0.62) C21 - C16 - Ir1 - C15
-160.47 (0.26) C15 - C16 - Ir1 - S1
82.90 (0.27) C12 - C16 - Ir1 - S1
-38.74 (0.52) C21 - C16 - Ir1 - S1
115.33 (0.56) C6 - C1 - Ir1 - C2
-126.77 (0.36) S1 - C1 - Ir1 - C2
175.31 (0.33) C2 - C1 - Ir1 - C16
-69.36 (0.61) C6 - C1 - Ir1 - C16
48.53 (0.45) S1 - C1 - Ir1 - C16
-152.91 (0.29) C2 - C1 - Ir1 - C12
-37.59 (0.51) C6 - C1 - Ir1 - C12
80.31 (0.23) S1 - C1 - Ir1 - C12
32.03 (0.29) C2 - C1 - Ir1 - C3
147.36 (0.51) C6 - C1 - Ir1 - C3
-94.75 (0.23) S1 - C1 - Ir1 - C3
-112.08 (0.30) C2 - C1 - Ir1 - C13
3.25 (0.49) C6 - C1 - Ir1 - C13
121.14 (0.20) S1 - C1 - Ir1 - C13
-74.58 (0.36) C2 - C1 - Ir1 - C14
40.75 (0.57) C6 - C1 - Ir1 - C14
158.64 (0.18) S1 - C1 - Ir1 - C14
-58.51 (1.01) C2 - C1 - Ir1 - C15
56.81 (1.15) C6 - C1 - Ir1 - C15
174.71 (0.82) S1 - C1 - Ir1 - C15
126.77 (0.36) C2 - C1 - Ir1 - S1
-117.90 (0.54) C6 - C1 - Ir1 - S1
54.55 (0.48) C13 - C12 - Ir1 - C2
172.12 (0.31) C16 - C12 - Ir1 - C2
-67.07 (0.64) C17 - C12 - Ir1 - C2

-117.56 (0.41) C13 - C12 - Ir1 - C16
120.82 (0.61) C17 - C12 - Ir1 - C16
87.49 (0.33) C13 - C12 - Ir1 - C1
-154.95 (0.27) C16 - C12 - Ir1 - C1
-34.13 (0.55) C17 - C12 - Ir1 - C1
-132.35 (1.45) C13 - C12 - Ir1 - C3
-14.79 (1.61) C16 - C12 - Ir1 - C3
106.03 (1.52) C17 - C12 - Ir1 - C3
117.56 (0.41) C16 - C12 - Ir1 - C13
-121.62 (0.64) C17 - C12 - Ir1 - C13
-37.90 (0.29) C13 - C12 - Ir1 - C14
79.67 (0.29) C16 - C12 - Ir1 - C14
-159.52 (0.56) C17 - C12 - Ir1 - C14
-79.70 (0.32) C13 - C12 - Ir1 - C15
37.86 (0.27) C16 - C12 - Ir1 - C15
158.68 (0.56) C17 - C12 - Ir1 - C15
132.75 (0.27) C13 - C12 - Ir1 - S1
-109.69 (0.25) C16 - C12 - Ir1 - S1
11.13 (0.52) C17 - C12 - Ir1 - S1
-118.41 (0.54) C4 - C3 - Ir1 - C2
172.88 (0.26) C2 - C3 - Ir1 - C16
54.46 (0.51) C4 - C3 - Ir1 - C16
-31.98 (0.28) C2 - C3 - Ir1 - C1
-150.40 (0.46) C4 - C3 - Ir1 - C1
-174.23 (1.39) C2 - C3 - Ir1 - C12
67.36 (1.64) C4 - C3 - Ir1 - C12
61.24 (0.47) C2 - C3 - Ir1 - C13
-57.18 (0.56) C4 - C3 - Ir1 - C13
94.88 (0.31) C2 - C3 - Ir1 - C14
-23.53 (0.46) C4 - C3 - Ir1 - C14
135.62 (0.29) C2 - C3 - Ir1 - C15
17.20 (0.46) C4 - C3 - Ir1 - C15
-77.72 (0.28) C2 - C3 - Ir1 - S1
163.87 (0.41) C4 - C3 - Ir1 - S1
-150.96 (0.30) C12 - C13 - Ir1 - C2
91.65 (0.30) C14 - C13 - Ir1 - C2
-28.27 (0.54) C18 - C13 - Ir1 - C2
38.05 (0.29) C12 - C13 - Ir1 - C16
-79.35 (0.29) C14 - C13 - Ir1 - C16
160.74 (0.53) C18 - C13 - Ir1 - C16

-109.70 (0.32) C12 - C13 - Ir1 - C1
132.90 (0.29) C14 - C13 - Ir1 - C1
12.99 (0.51) C18 - C13 - Ir1 - C1
-117.40 (0.42) C14 - C13 - Ir1 - C12
122.69 (0.61) C18 - C13 - Ir1 - C12
170.39 (0.33) C12 - C13 - Ir1 - C3
52.99 (0.46) C14 - C13 - Ir1 - C3
-66.92 (0.62) C18 - C13 - Ir1 - C3
117.40 (0.42) C12 - C13 - Ir1 - C14
-119.91 (0.59) C18 - C13 - Ir1 - C14
80.63 (0.32) C12 - C13 - Ir1 - C15
-36.76 (0.26) C14 - C13 - Ir1 - C15
-156.68 (0.54) C18 - C13 - Ir1 - C15
-61.90 (0.33) C12 - C13 - Ir1 - S1
-179.29 (0.21) C14 - C13 - Ir1 - S1
60.79 (0.51) C18 - C13 - Ir1 - S1
134.03 (0.29) C15 - C14 - Ir1 - C2
-107.99 (0.29) C13 - C14 - Ir1 - C2
11.43 (0.50) C19 - C14 - Ir1 - C2
-37.06 (0.27) C15 - C14 - Ir1 - C16
80.92 (0.30) C13 - C14 - Ir1 - C16
-159.67 (0.52) C19 - C14 - Ir1 - C16
174.78 (0.27) C15 - C14 - Ir1 - C1
-67.24 (0.37) C13 - C14 - Ir1 - C1
52.17 (0.53) C19 - C14 - Ir1 - C1
-80.48 (0.31) C15 - C14 - Ir1 - C12
37.51 (0.28) C13 - C14 - Ir1 - C12
156.92 (0.50) C19 - C14 - Ir1 - C12
91.54 (0.31) C15 - C14 - Ir1 - C3
-150.48 (0.28) C13 - C14 - Ir1 - C3
-31.07 (0.51) C19 - C14 - Ir1 - C3
-117.99 (0.39) C15 - C14 - Ir1 - C13
119.41 (0.57) C19 - C14 - Ir1 - C13
117.99 (0.39) C13 - C14 - Ir1 - C15
-122.60 (0.55) C19 - C14 - Ir1 - C15
-115.89 (0.43) C15 - C14 - Ir1 - S1
2.10 (0.62) C13 - C14 - Ir1 - S1
121.51 (0.49) C19 - C14 - Ir1 - S1
-68.08 (0.37) C14 - C15 - Ir1 - C2
173.06 (0.28) C16 - C15 - Ir1 - C2

52.37 (0.58) C20 - C15 - Ir1 - C2
118.86 (0.41) C14 - C15 - Ir1 - C16
-120.68 (0.61) C20 - C15 - Ir1 - C16
-19.92 (1.03) C14 - C15 - Ir1 - C1
-138.78 (0.88) C16 - C15 - Ir1 - C1
100.53 (1.02) C20 - C15 - Ir1 - C1
80.32 (0.29) C14 - C15 - Ir1 - C12
-38.54 (0.29) C16 - C15 - Ir1 - C12
-159.23 (0.53) C20 - C15 - Ir1 - C12
-105.80 (0.29) C14 - C15 - Ir1 - C3
135.33 (0.30) C16 - C15 - Ir1 - C3
14.65 (0.53) C20 - C15 - Ir1 - C3
37.76 (0.27) C14 - C15 - Ir1 - C13
-81.10 (0.31) C16 - C15 - Ir1 - C13
158.21 (0.54) C20 - C15 - Ir1 - C13
-118.86 (0.41) C16 - C15 - Ir1 - C14
120.45 (0.57) C20 - C15 - Ir1 - C14
153.28 (0.23) C14 - C15 - Ir1 - S1
34.42 (0.43) C16 - C15 - Ir1 - S1
-86.26 (0.50) C20 - C15 - Ir1 - S1
2.64 (0.73) C3 - C4 - N1 - C7
178.92 (0.47) C5 - C4 - N1 - C7
-164.96 (0.46) C3 - C4 - N1 - C11
11.31 (0.70) C5 - C4 - N1 - C11
144.04 (0.52) C8 - C7 - N1 - C4
-47.46 (0.67) C8 - C7 - N1 - C11
-144.00 (0.58) C10 - C11 - N1 - C4
47.73 (0.70) C10 - C11 - N1 - C7
-57.04 (0.32) C2 - C1 - S1 - Ir1
122.94 (0.47) C6 - C1 - S1 - Ir1
31.40 (0.25) C2 - Ir1 - S1 - C1
-155.95 (0.26) C16 - Ir1 - S1 - C1
-116.38 (0.26) C12 - Ir1 - S1 - C1
70.92 (0.25) C3 - Ir1 - S1 - C1
-82.55 (0.28) C13 - Ir1 - S1 - C1
-84.15 (0.47) C14 - Ir1 - S1 - C1
-178.07 (0.30) C15 - Ir1 - S1 - C1

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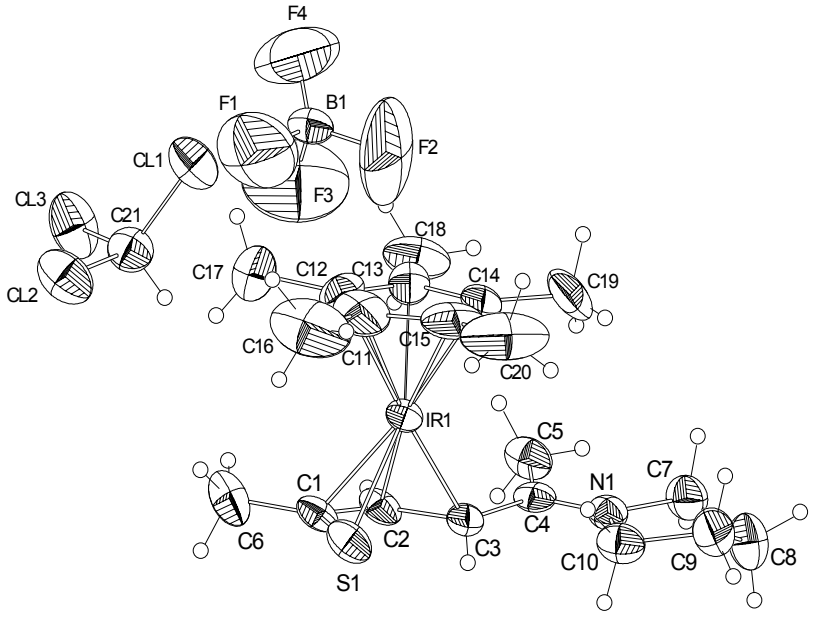

ORTEP drawing of Compound **13**

Formula: C_{21} H_{32} B Cl_3 F_4 Ir N S

Authors : Marisol Cervantes Vásquez y Ma. de los Ángeles Paz Sandoval.

Tab. 1 Crystal data and data collection
Tab. 2 Solution and refinement
Tab. 3 Atomic coordinates and equivalent isotropic displacement parameters
Tab. 4 Bond lengths and angles
Tab. 5 Anisotropic displacement parameters
Tab. 6 Hydrogen coordinates and isotropic displacement parameters

Table 1. Crystal data and data collection

Identification code	Compound **13**	
Operator	MLR and BPM	
Empirical formula	C_{21} H_{32} B Cl_3 F_4 Ir N S	
Formula weight	715.90	
Crystal size	0.56 x 0.45 x 0.33 mm	
Crystal color and habit	red prism	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 9.6363(10) Å	α = 67.321(10)°
	b = 12.0380(10) Å	β = 74.241(10)°
	c = 12.6614(10) Å	γ = 85.072(10)°
Volume	1304.0(2) $Å^3$	
Z	2	
Density (calculated)	1.823 Mg/m^3	
Absorption coefficient	5.546 mm^{-1}	
F(000)	700	
Diffractometer used	Enraf-Nonius CAD4	
Radiation and wavelength	MoKα with λ=0.71073 Å	
Scan type	ω/2θ	
Temperature	293(2) K	
2θ range for data collection	5.32 to 52.48°	
Index ranges	$-11 \le h \le 11$ $-13 \le k \le 14$ $0 \le l \le 15$	
Reflections collected	2932	
Independent reflections	2932 (R_{int} = 0.0000)	
Observed reflections	2932 (F>4σ(F))	
Absorption correction	Semi-empirical	
Max. and min. transmission	0.7685 and 0.234	

Experimental details :

Scan speed	Variable; 16.1 to 60 °/min in ω
Scan range (ω)	0.7 °

Background measurement : Moving crystal and moving counter at the beginning and end of scan, each for 25% of total scan area.

Crystal mounted in perfluorpolyether oil

Table 2. Solution and refinement

Structure solution program	SHELXS-97(Sheldrick 1990)
Solution	heavy-atom-method
Refinement method	Full-matrix Least-Squares on F^2
Hydrogen atoms	mixed
Weighting scheme	$w^{-1}=\sigma^2Fo^2+(P)^2+P$ where $P=(Fo^2+2Fc^2)/3$
Data / restraints / parameters	2932 / 0 / 298
Data-to-parameter-ratio	9.8 : 1 (9.8 : 1 [F>4σ(F)])
Final R indices [F>4σ(F)]	R1 = 0.0391, wR2 = 0.1037
R indices (all data)	R1 = 0.0391, wR2 = 0.1037
Goodness-of-Fit on F^2	1.056
Largest and mean Δ/σ	0.001 0.000
Largest difference peak	1.590 eÅ^{-3}
Largest difference hole	-1.158 eÅ^{-3}

Refinement details :

Program used	SHELXL-97 (Sheldrick 1997)
CifRtf version used	2.0

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for compound **13.** U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U(eq)
C(1)	4926(10)	7251(9)	7410(8)	36(3)
C(2)	5699(11)	8270(7)	6472(8)	39(3)
C(3)	5673(12)	8408(10)	5276(8)	39(3)
C(4)	6631(10)	9232(7)	4253(7)	34(3)
C(5)	7723(13)	9992(9)	4292(9)	49(3)
C(6)	4925(15)	6984(10)	8653(8)	57(4)
C(7)	7341(13)	10121(10)	2081(9)	51(3)
C(8)	6572(17)	9993(11)	1237(9)	60(4)
C(9)	6018(16)	8719(11)	1785(9)	60(4)
C(10)	5560(13)	8520(9)	3097(9)	48(3)
C(11)	7356(17)	4871(10)	6848(12)	77(6)
C(12)	8092(14)	5617(10)	7090(9)	50(4)
C(13)	8838(11)	6506(10)	6103(11)	46(3)
C(14)	8530(13)	6311(10)	5093(8)	53(4)
C(15)	7602(15)	5312(12)	5558(13)	67(4)
C(16)	6420(02)	3772(12)	7628(18)	120(9)
C(17)	8200(02)	5428(18)	8320(11)	98(7)
C(18)	9814(15)	7466(13)	5935(14)	76(5)
C(19)	9185(19)	7055(17)	3811(11)	122(9)
C(20)	7116(19)	4759(17)	4857(19)	122(9)
C(21)	9468(14)	7396(10)	9943(10)	52(3)
Ir(1)	6531.6(4)	6673.4(3)	6191.0(3)	29.5(1)
S(1)	4006(3)	6358(2)	7016(2)	46.5(8)
N(1)	6503(9)	9295(6)	3231(6)	39(2)
Cl(1)	10853(4)	6868(3)	9065(3)	63.9(10)
Cl(2)	8258(4)	6228(3)	10924(3)	70.9(11)
Cl(3)	10167(5)	8054(3)	10699(3)	76.6(13)
B(1)	8120(14)	96(12)	7757(11)	46(4)
F(1)	7123(17)	-803(14)	8556(13)	169(7)
F(2)	7920(02)	360(18)	6693(10)	191(8)
F(3)	7590(02)	1007(14)	7945(18)	206(9)
F(4)	9262(15)	-106(19)	7937(14)	234(13)

Table 4. Bond lengths [Å] and angles [°] for compound **13**

C(1)-C(2)	1.422(14)	C(1)-C(6)	1.480(14)
C(1)-S(1)	1.734(11)	C(1)-Ir(1)	2.146(7)
C(2)-C(3)	1.465(13)	C(2)-Ir(1)	2.138(7)
C(3)-C(4)	1.426(14)		
C(3)-Ir(1)	2.178(9)	C(3)-H(3)	0.78(11)
C(4)-N(1)	1.306(12)	C(4)-C(5)	1.474(17)
C(7)-N(1)	1.464(12)	C(7)-C(8)	1.51(2)
C(8)-C(9)	1.496(18)	C(9)-C(10)	1.525(15)
C(10)-N(1)	1.441(16)	C(11)-C(12)	1.36(2)
C(11)-C(15)	1.465(19)	C(11)-C(16)	1.50(2)
C(11)-Ir(1)	2.169(9)	C(12)-C(13)	1.355(17)
C(12)-C(17)	1.516(17)	C(12)-Ir(1)	2.158(10)
C(13)-C(18)	1.47(2)	C(13)-C(14)	1.493(16)
C(13)-Ir(1)	2.191(10)	C(14)-C(15)	1.394(19)
C(14)-C(19)	1.501(15)	C(14)-Ir(1)	2.168(8)
C(15)-C(20)	1.478(18)	C(15)-Ir(1)	2.160(9)
C(21)-Cl(1)	1.736(10)	C(21)-Cl(3)	1.739(14)
C(21)-Cl(2)	1.740(14)	Ir(1)-S(1)	2.372(3)
B(1)-F(4)	1.17(2)	B(1)-F(3)	1.250(17)
B(1)-F(2)	1.324(17)	B(1)-F(1)	1.39(2)
C(2)-C(1)-C(6)	120.7(10)	C(2)-C(1)-S(1)	116.7(7)
C(6)-C(1)-S(1)	122.6(9)	C(2)-C(1)-Ir(1)	70.3(4)
C(6)-C(1)-Ir(1)	125.0(7)	S(1)-C(1)-Ir(1)	74.5(3)
C(1)-C(2)-C(3)	115.6(10)	C(1)-C(2)-Ir(1)	70.9(4)
C(3)-C(2)-Ir(1)	71.6(5)	C(4)-C(3)-C(2)	121.2(12)
C(4)-C(3)-Ir(1)	117.2(6)	C(2)-C(3)-Ir(1)	68.7(4)
C(4)-C(3)-H(3)	115(6)	C(2)-C(3)-H(3)	110(6)
Ir(1)-C(3)-H(3)	117(7)	N(1)-C(4)-C(3)	116.1(10)
N(1)-C(4)-C(5)	119.7(9)	C(3)-C(4)-C(5)	124.2(9)
N(1)-C(7)-C(8)	102.2(11)	C(9)-C(8)-C(7)	105.4(9)
C(8)-C(9)-C(10)	101.5(10)	N(1)-C(10)-C(9)	105.2(10)
C(12)-C(11)-C(15)	107.6(12)	C(12)-C(11)-C(16)	132.4(16)
C(15)-C(11)-C(16)	120.1(18)	C(12)-C(11)-Ir(1)	71.3(5)
C(15)-C(11)-Ir(1)	69.9(5)	C(16)-C(11)-Ir(1)	123.9(10)
C(13)-C(12)-C(11)	113.1(11)	C(13)-C(12)-C(17)	122.3(15)
C(11)-C(12)-C(17)	124.4(14)	C(13)-C(12)-Ir(1)	73.2(5)
C(11)-C(12)-Ir(1)	72.1(7)	C(17)-C(12)-Ir(1)	127.2(8)
C(12)-C(13)-C(18)	132.1(12)	C(12)-C(13)-C(14)	105.1(11)

C(18)-C(13)-C(14)	122.8(12)	C(12)-C(13)-Ir(1)	70.5(7)
C(18)-C(13)-Ir(1)	126.1(7)	C(14)-C(13)-Ir(1)	69.2(6)
C(15)-C(14)-C(13)	108.1(10)	C(15)-C(14)-C(19)	127.7(15)
C(13)-C(14)-C(19)	124.2(15)	C(15)-C(14)-Ir(1)	70.9(6)
C(13)-C(14)-Ir(1)	70.8(5)	C(19)-C(14)-Ir(1)	126.0(7)
C(14)-C(15)-C(11)	106.1(12)	C(14)-C(15)-C(20)	125.5(15)
C(11)-C(15)-C(20)	128.1(17)	C(14)-C(15)-Ir(1)	71.5(5)
C(11)-C(15)-Ir(1)	70.5(5)	C(20)-C(15)-Ir(1)	127.5(8)
C(11)-C(16)-H(16A)	109.5	Cl(1)-C(21)-Cl(3)	110.2(8)
Cl(1)-C(21)-Cl(2)	110.1(6)	Cl(3)-C(21)-Cl(2)	111.1(6)
C(2)-Ir(1)-C(1)	38.8(4)		
C(2)-Ir(1)-C(12)	120.5(4)	C(1)-Ir(1)-C(12)	108.8(4)
C(2)-Ir(1)-C(15)	168.4(5)	C(1)-Ir(1)-C(15)	152.6(5)
C(12)-Ir(1)-C(15)	63.7(5)	C(2)-Ir(1)-C(14)	132.5(5)
C(1)-Ir(1)-C(14)	165.1(5)	C(12)-Ir(1)-C(14)	63.1(4)
C(15)-Ir(1)-C(14)	37.6(5)	C(2)-Ir(1)-C(11)	150.0(5)
C(1)-Ir(1)-C(11)	118.3(4)	C(12)-Ir(1)-C(11)	36.6(6)
C(15)-Ir(1)-C(11)	39.6(5)	C(14)-Ir(1)-C(11)	63.6(4)
C(2)-Ir(1)-C(3)	39.7(4)	C(1)-Ir(1)-C(3)	68.8(3)
C(12)-Ir(1)-C(3)	150.8(5)	C(15)-Ir(1)-C(3)	131.3(4)
C(14)-Ir(1)-C(3)	111.6(3)	C(11)-Ir(1)-C(3)	170.1(5)
C(2)-Ir(1)-C(13)	111.3(4)	C(1)-Ir(1)-C(13)	126.0(4)
C(12)-Ir(1)-C(13)	36.3(4)	C(15)-Ir(1)-C(13)	65.0(5)
C(14)-Ir(1)-C(13)	40.0(4)	C(11)-Ir(1)-C(13)	62.6(6)
C(3)-Ir(1)-C(13)	120.1(5)	C(2)-Ir(1)-S(1)	73.1(3)
C(1)-Ir(1)-S(1)	44.8(3)	C(12)-Ir(1)-S(1)	122.8(3)
C(15)-Ir(1)-S(1)	114.7(4)	C(14)-Ir(1)-S(1)	149.9(4)
C(11)-Ir(1)-S(1)	102.7(4)	C(3)-Ir(1)-S(1)	77.2(3)
C(13)-Ir(1)-S(1)	158.6(3)	C(1)-S(1)-Ir(1)	60.7(3)
C(4)-N(1)-C(10)	124.0(8)	C(4)-N(1)-C(7)	124.4(10)
C(10)-N(1)-C(7)	111.5(9)	F(4)-B(1)-F(3)	112(2)
F(4)-B(1)-F(2)	122.1(16)	F(3)-B(1)-F(2)	99.4(14)
F(4)-B(1)-F(1)	111.5(13)	F(3)-B(1)-F(1)	102.3(14)
F(2)-B(1)-F(1)	107.3(16)		

Table 5. Anisotropic displacement parameters [$Å^2 \times 10^3$]

	U11	U22	U33	U23	U13	U12
C(1)	22(5)	47(5)	47(5)	-29(4)	0(4)	-5(5)
C(2)	41(6)	27(4)	48(5)	-22(4)	1(4)	9(5)
C(3)	37(6)	39(5)	35(4)	-13(4)	-6(4)	14(6)
C(4)	30(5)	18(3)	48(5)	-11(3)	-8(4)	7(4)
C(5)	39(7)	37(5)	60(6)	-13(4)	-1(5)	-4(6)
C(6)	66(10)	50(5)	43(5)	-19(4)	12(6)	-13(7)
C(7)	44(7)	45(5)	46(5)	-5(4)	-1(5)	-6(7)
C(8)	67(11)	60(7)	45(5)	-15(5)	-4(6)	-15(9)
C(9)	63(9)	64(7)	49(5)	-22(5)	-9(6)	8(8)
C(10)	36(7)	42(5)	62(6)	-17(5)	-8(5)	-5(6)
C(11)	81(11)	30(5)	91(9)	-8(5)	-2(8)	27(7)
C(12)	57(8)	45(6)	48(5)	-14(4)	-23(5)	17(7)
C(13)	17(5)	56(6)	90(8)	-45(6)	-28(5)	8(6)
C(14)	49(7)	61(7)	45(5)	-24(5)	-8(5)	33(7)
C(15)	58(9)	62(7)	114(10)	-67(8)	-38(8)	34(8)
C(16)	91(15)	36(6)	171(17)	-2(8)	10(13)	1(10)
C(17)	98(14)	139(15)	56(7)	-34(9)	-31(8)	34(14)
C(18)	39(8)	86(10)	120(11)	-56(9)	-24(8)	6(9)
C(19)	106(14)	149(16)	54(7)	-22(8)	21(8)	73(14)
C(20)	96(15)	168(18)	230(02)	-179(18)	-100(15)	70(15)
C(21)	55(8)	45(5)	58(6)	-23(5)	-14(6)	5(7)
Ir(1)	27.5(2)	26.6(1)	37.1(1)	-16.4(1)	-6.3(1)	1.2(1)
S(1)	33.2(16)	46.4(13)	53.2(13)	-20.2(11)	5.5(12)	-11.9(15)
N(1)	36(5)	30(3)	44(4)	-12(3)	-7(4)	7(4)
Cl(1)	59(2)	68.8(17)	66.3(16)	-38.3(14)	0.6(15)	-5(2)
Cl(2)	62(2)	58.1(16)	83(2)	-31.1(15)	5.1(18)	-11(2)
Cl(3)	87(3)	86(2)	67.2(17)	-45.9(16)	-1(2)	-27(3)
B(1)	30(7)	49(6)	57(6)	-21(5)	-8(6)	3(7)
F(1)	106(13)	165(12)	174(12)	-16(10)	2(10)	-29(13)
F(2)	190(02)	330(02)	82(7)	-69(10)	-53(10)	-100(02)
F(3)	210(02)	150(12)	320(02)	-148(15)	-87(18)	40(15)
F(4)	86(10)	260(02)	183(13)	78(13)	-21(9)	39(14)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for compound **13**

	x	y	z	U(eq)
H(2)	6289	8798	6611	47
H(5A)	8391	9492	4704	80
H(5B)	7250	10504	4699	80
H(5C)	8234	10478	3499	80
H(6A)	4928	6130	9082	80
H(6B)	4101	7320	9042	80
H(6C)	5790	7344	8630	80
H(7A)	8325	9876	1917	80
H(7B)	7329	10932	2047	80
H(8A)	7256	10141	484	80
H(8B)	5812	10563	1130	80
H(9A)	6739	8160	1629	80
H(9B)	5202	8648	1515	80
H(10A)	5664	7694	3582	80
H(10B)	4572	8734	3323	80
H(16A)	6917	3226	8181	179
H(16B)	6221	3384	7149	179
H(16C)	5536	4002	8052	179
H(17A)	8840	4781	8568	147
H(17B)	7260	5232	8865	147
H(17C)	8562	6153	8306	147
H(18A)	9270	8050	6213	114
H(18B)	10289	7847	5108	114
H(18C)	10521	7128	6373	114
H(19A)	8728	6845	3326	183
H(19B)	10198	6902	3612	183
H(19C)	9048	7893	3676	183
H(20A)	6873	5381	4188	183
H(20B)	6283	4252	5343	183
H(20C)	7875	4286	4586	183
H(21)	8966	7996	9435	80
H(3)	4880(101)	8410(08)	5240(06)	10(02)

Table 7. Crystal data and data collection parameters

Compound	Compound **13**
Chem. formula	C_{21} H_{32} B Cl_3 F_4 Ir N S
Form. wght.	715.90
Cryst. size [mm]	0.33x0.45x0.56
Cryst. system	Triclinic
Space group	P –1
a, [Å]	9.6363(10)
b, [Å]	12.0380(10)
c, [Å]	12.6614(10)
α, [°]	67.321(10)
β, [°]	74.241(10)
γ, [°]	85.072(10)
V, [Å^3]	1304.0(2)
Z	2
ρ(calcd.), [Mg/m^3]	1.823
μ [mm^{-1}]	5.546
F(000)	700
Index range	-11≤h≤11-13≤k≤140≤l≤15
2 θ [°]	52.48
Temp, [K]	293(2)
Refl. collected	2932
Refl. unique	2932
Refl. observed (4σ)	2932
R (int.)	0.0000
No. variables	298
Weighting scheme[1] x/y	/
GOOF	1.056
Final R (4σ)	0.0391
Final wR2	0.1037
Larg. res. peak [e/Å^3]	1.590

[1] $w^{-1} = \sigma^2 F_o^2 + (xP)^2 + yP$; $P = (F_o^2 + 2F_c^2)/3$

Selected torsion angles for compound 13

177.25 (0.80) C6 - C1 - C2 - C3
-2.37 (0.95) S1 - C1 - C2 - C3
57.76 (0.60) Ir1 - C1 - C2 - C3
119.49 (0.84) C6 - C1 - C2 - Ir1
-60.13 (0.48) S1 - C1 - C2 - Ir1
-166.97 (0.70) C1 - C2 - C3 - C4
-109.60 (0.71) Ir1 - C2 - C3 - C4
-57.37 (0.60) C1 - C2 - C3 - Ir1
-179.32 (0.66) C2 - C3 - C4 - N1
100.46 (0.85) Ir1 - C3 - C4 - N1
0.65 (1.15) C2 - C3 - C4 - C5
-79.57 (0.98) Ir1 - C3 - C4 - C5
-32.04 (1.07) N1 - C7 - C8 - C9
37.72 (1.21) C7 - C8 - C9 - C10
-28.92 (1.13) C8 - C9 - C10 - N1
-176.62 (0.97) C16 - C11 - C12 - C13
0.46 (1.06) C15 - C11 - C12 - C13
61.43 (0.81) Ir1 - C11 - C12 - C13
-1.95 (1.55) C16 - C11 - C12 - C17
175.14 (0.92) C15 - C11 - C12 - C17
-123.89 (0.97) Ir1 - C11 - C12 - C17
121.94 (0.99) C16 - C11 - C12 - Ir1
-60.97 (0.53) C15 - C11 - C12 - Ir1
-1.17 (1.20) C11 - C12 - C13 - C14
-175.65 (0.98) C17 - C12 - C13 - C14
60.86 (0.69) Ir1 - C12 - C13 - C14
177.81 (1.15) C11 - C12 - C13 - C18
3.33 (2.00) C17 - C12 - C13 - C18
-120.17 (1.35) Ir1 - C12 - C13 - C18
-62.02 (0.71) C11 - C12 - C13 - Ir1
123.49 (1.09) C17 - C12 - C13 - Ir1
1.40 (1.11) C12 - C13 - C14 - C15
-177.72 (1.01) C18 - C13 - C14 - C15
63.16 (0.63) Ir1 - C13 - C14 - C15
175.05 (1.05) C12 - C13 - C14 - C19
-4.06 (1.72) C18 - C13 - C14 - C19
-123.19 (1.15) Ir1 - C13 - C14 - C19
-61.76 (0.71) C12 - C13 - C14 - Ir1

119.12 (1.15) C18 - C13 - C14 - Ir1
-1.12 (0.95) C13 - C14 - C15 - C11
-174.88 (0.94) C19 - C14 - C15 - C11
61.33 (0.55) Ir1 - C14 - C15 - C11
175.69 (0.92) C13 - C14 - C15 - C20
1.92 (1.62) C19 - C14 - C15 - C20
-121.86 (0.97) Ir1 - C14 - C15 - C20
-62.45 (0.63) C13 - C14 - C15 - Ir1
123.79 (1.09) C19 - C14 - C15 - Ir1
0.47 (0.91) C12 - C11 - C15 - C14
177.85 (0.83) C16 - C11 - C15 - C14
-61.34 (0.62) Ir1 - C11 - C15 - C14
-176.49 (0.87) C12 - C11 - C15 - C20
0.89 (1.29) C16 - C11 - C15 - C20
121.70 (0.86) Ir1 - C11 - C15 - C20
61.81 (0.59) C12 - C11 - C15 - Ir1
-120.81 (0.84) C16 - C11 - C15 - Ir1
-126.50 (0.99) C3 - C2 - Ir1 - C1
-82.33 (0.77) C1 - C2 - Ir1 - C12
151.17 (0.71) C3 - C2 - Ir1 - C12
169.81 (2.02) C1 - C2 - Ir1 - C14
43.31 (2.44) C3 - C2 - Ir1 - C14
-49.93 (1.32) C1 - C2 - Ir1 - C13
-176.43 (0.99) C3 - C2 - Ir1 - C13
-162.24 (0.61) C1 - C2 - Ir1 - C15
71.26 (0.87) C3 - C2 - Ir1 - C15
126.50 (0.99) C1 - C2 - Ir1 - C3
-121.67 (0.68) C1 - C2 - Ir1 - C11
111.83 (0.73) C3 - C2 - Ir1 - C11
36.28 (0.56) C1 - C2 - Ir1 - S1
-90.22 (0.67) C3 - C2 - Ir1 - S1
-114.33 (1.29) C6 - C1 - Ir1 - C2
126.54 (0.73) S1 - C1 - Ir1 - C2
115.50 (0.71) C2 - C1 - Ir1 - C12
1.17 (1.15) C6 - C1 - Ir1 - C12
-117.96 (0.47) S1 - C1 - Ir1 - C12
-175.52 (0.86) C2 - C1 - Ir1 - C14
70.16 (1.48) C6 - C1 - Ir1 - C14
-48.97 (1.04) S1 - C1 - Ir1 - C14
154.25 (0.79) C2 - C1 - Ir1 - C13

39.92 (1.23) C6 - C1 - Ir1 - C13
-79.20 (0.66) S1 - C1 - Ir1 - C13
60.69 (1.47) C2 - C1 - Ir1 - C15
-53.63 (1.78) C6 - C1 - Ir1 - C15
-172.76 (1.11) S1 - C1 - Ir1 - C15
-33.43 (0.68) C2 - C1 - Ir1 - C3
-147.76 (1.15) C6 - C1 - Ir1 - C3
93.11 (0.51) S1 - C1 - Ir1 - C3
78.92 (0.75) C2 - C1 - Ir1 - C11
-35.41 (1.18) C6 - C1 - Ir1 - C11
-154.54 (0.43) S1 - C1 - Ir1 - C11
-126.54 (0.73) C2 - C1 - Ir1 - S1
119.13 (1.10) C6 - C1 - Ir1 - S1
153.29 (0.71) C13 - C12 - Ir1 - C2
-84.76 (0.71) C11 - C12 - Ir1 - C2
32.70 (1.59) C17 - C12 - Ir1 - C2
112.34 (0.77) C13 - C12 - Ir1 - C1
-125.71 (0.68) C11 - C12 - Ir1 - C1
-8.26 (1.57) C17 - C12 - Ir1 - C1
-39.13 (0.80) C13 - C12 - Ir1 - C14
82.81 (0.80) C11 - C12 - Ir1 - C14
-159.73 (1.64) C17 - C12 - Ir1 - C14
121.94 (1.02) C11 - C12 - Ir1 - C13
-120.60 (1.77) C17 - C12 - Ir1 - C13
-81.36 (0.83) C13 - C12 - Ir1 - C15
40.59 (0.70) C11 - C12 - Ir1 - C15
158.04 (1.63) C17 - C12 - Ir1 - C15
-167.61 (0.69) C13 - C12 - Ir1 - C3
-45.66 (1.03) C11 - C12 - Ir1 - C3
71.79 (1.67) C17 - C12 - Ir1 - C3
-121.94 (1.02) C13 - C12 - Ir1 - C11
117.46 (1.74) C17 - C12 - Ir1 - C11
64.54 (0.79) C13 - C12 - Ir1 - S1
-173.52 (0.53) C11 - C12 - Ir1 - S1
-56.06 (1.56) C17 - C12 - Ir1 - S1
34.58 (2.51) C15 - C14 - Ir1 - C2
149.93 (2.04) C13 - C14 - Ir1 - C2
-87.28 (2.87) C19 - C14 - Ir1 - C2
-159.39 (0.79) C15 - C14 - Ir1 - C1
-44.04 (1.44) C13 - C14 - Ir1 - C1

78.75 (1.92) C19 - C14 - Ir1 - C1
-79.21 (0.77) C15 - C14 - Ir1 - C12
36.14 (0.88) C13 - C14 - Ir1 - C12
158.92 (1.83) C19 - C14 - Ir1 - C12
-115.35 (1.18) C15 - C14 - Ir1 - C13
122.78 (2.10) C19 - C14 - Ir1 - C13
115.35 (1.18) C13 - C14 - Ir1 - C15
-121.87 (1.94) C19 - C14 - Ir1 - C15
70.23 (0.94) C15 - C14 - Ir1 - C3
-174.42 (0.85) C13 - C14 - Ir1 - C3
-51.64 (1.91) C19 - C14 - Ir1 - C3
-38.67 (0.67) C15 - C14 - Ir1 - C11
76.67 (0.93) C13 - C14 - Ir1 - C11
-160.54 (1.82) C19 - C14 - Ir1 - C11
164.79 (0.56) C15 - C14 - Ir1 - S1
-79.86 (0.93) C13 - C14 - Ir1 - S1
42.92 (1.74) C19 - C14 - Ir1 - S1
-50.80 (1.35) C12 - C13 - Ir1 - C2
-168.28 (0.85) C14 - C13 - Ir1 - C2
77.74 (2.13) C18 - C13 - Ir1 - C2
-83.75 (0.85) C12 - C13 - Ir1 - C1
158.77 (0.80) C14 - C13 - Ir1 - C1
44.79 (1.82) C18 - C13 - Ir1 - C1
-117.48 (1.21) C14 - C13 - Ir1 - C12
128.54 (1.92) C18 - C13 - Ir1 - C12
117.48 (1.21) C12 - C13 - Ir1 - C14
-113.98 (2.08) C18 - C13 - Ir1 - C14
79.53 (0.83) C12 - C13 - Ir1 - C15
-37.95 (0.82) C14 - C13 - Ir1 - C15
-151.93 (1.84) C18 - C13 - Ir1 - C15
142.56 (2.61) C12 - C13 - Ir1 - C3
25.08 (3.29) C14 - C13 - Ir1 - C3
-88.90 (2.89) C18 - C13 - Ir1 - C3
34.54 (0.70) C12 - C13 - Ir1 - C11
-82.94 (0.90) C14 - C13 - Ir1 - C11
163.08 (1.80) C18 - C13 - Ir1 - C11
-128.95 (0.69) C12 - C13 - Ir1 - S1
113.57 (0.84) C14 - C13 - Ir1 - S1
-0.41 (1.69) C18 - C13 - Ir1 - S1
-171.04 (0.67) C14 - C15 - Ir1 - C2

70.85 (0.75) C11 - C15 - Ir1 - C2
-47.80 (1.73) C20 - C15 - Ir1 - C2
141.31 (1.35) C14 - C15 - Ir1 - C1
23.20 (1.57) C11 - C15 - Ir1 - C1
-95.45 (1.85) C20 - C15 - Ir1 - C1
81.13 (0.80) C14 - C15 - Ir1 - C12
-36.98 (0.66) C11 - C15 - Ir1 - C12
-155.63 (1.72) C20 - C15 - Ir1 - C12
-118.11 (0.94) C11 - C15 - Ir1 - C14
123.24 (1.85) C20 - C15 - Ir1 - C14
40.03 (0.83) C14 - C15 - Ir1 - C13
-78.09 (0.79) C11 - C15 - Ir1 - C13
163.26 (1.74) C20 - C15 - Ir1 - C13
-130.46 (0.77) C14 - C15 - Ir1 - C3
111.42 (0.70) C11 - C15 - Ir1 - C3
-7.23 (1.67) C20 - C15 - Ir1 - C3
118.11 (0.94) C14 - C15 - Ir1 - C11
-118.65 (1.81) C20 - C15 - Ir1 - C11
-28.46 (0.96) C14 - C15 - Ir1 - S1
-146.58 (0.60) C11 - C15 - Ir1 - S1
94.77 (1.60) C20 - C15 - Ir1 - S1
114.96 (1.29) C4 - C3 - Ir1 - C2
147.62 (1.07) C4 - C3 - Ir1 - C1
32.66 (0.64) C2 - C3 - Ir1 - C1
56.66 (1.20) C4 - C3 - Ir1 - C12
-58.29 (0.98) C2 - C3 - Ir1 - C12
-54.39 (1.27) C4 - C3 - Ir1 - C14
-169.35 (0.70) C2 - C3 - Ir1 - C14
-75.45 (3.18) C4 - C3 - Ir1 - C13
169.59 (2.63) C2 - C3 - Ir1 - C13
-16.30 (1.09) C4 - C3 - Ir1 - C15
-131.26 (0.70) C2 - C3 - Ir1 - C15
27.32 (1.06) C4 - C3 - Ir1 - C11
-87.64 (0.69) C2 - C3 - Ir1 - C11
-166.20 (0.95) C4 - C3 - Ir1 - S1
78.84 (0.61) C2 - C3 - Ir1 - S1
113.01 (0.69) C12 - C11 - Ir1 - C2
-14.67 (1.23) C16 - C11 - Ir1 - C2
-131.58 (0.62) C15 - C11 - Ir1 - C2
71.82 (0.80) C12 - C11 - Ir1 - C1

-55.86 (1.29) C16 - C11 - Ir1 - C1
-172.77 (0.56) C15 - C11 - Ir1 - C1
-127.68 (1.44) C16 - C11 - Ir1 - C12
115.41 (0.96) C15 - C11 - Ir1 - C12
-79.00 (0.79) C12 - C11 - Ir1 - C14
153.32 (1.32) C16 - C11 - Ir1 - C14
36.41 (0.65) C15 - C11 - Ir1 - C14
-34.69 (0.71) C12 - C11 - Ir1 - C13
-162.37 (1.33) C16 - C11 - Ir1 - C13
80.72 (0.75) C15 - C11 - Ir1 - C13
-115.41 (0.96) C12 - C11 - Ir1 - C15
116.91 (1.41) C16 - C11 - Ir1 - C15
156.22 (0.66) C12 - C11 - Ir1 - C3
28.53 (1.28) C16 - C11 - Ir1 - C3
-88.37 (0.70) C15 - C11 - Ir1 - C3
15.16 (1.23) C12 - C11 - Ir1 - S1
-112.52 (1.21) C16 - C11 - Ir1 - S1
130.57 (0.77) C15 - C11 - Ir1 - S1
57.91 (0.54) C2 - C1 - S1 - Ir1
-121.70 (0.83) C6 - C1 - S1 - Ir1
-31.70 (0.44) C2 - Ir1 - S1 - C1
84.09 (0.53) C12 - Ir1 - S1 - C1
157.61 (0.56) C14 - Ir1 - S1 - C1
117.56 (0.58) C13 - Ir1 - S1 - C1
176.27 (0.55) C15 - Ir1 - S1 - C1
-72.62 (0.47) C3 - Ir1 - S1 - C1
73.44 (0.88) C11 - Ir1 - S1 - C1
-5.53 (1.01) C3 - C4 - N1 - C10
174.49 (0.73) C5 - C4 - N1 - C10
177.22 (0.72) C3 - C4 - N1 - C7
-2.76 (1.07) C5 - C4 - N1 - C7
-167.61 (0.73) C9 - C10 - N1 - C4
9.96 (0.94) C9 - C10 - N1 - C7
-169.21 (0.77) C8 - C7 - N1 - C4
13.24 (0.97) C8 - C7 - N1 - C10

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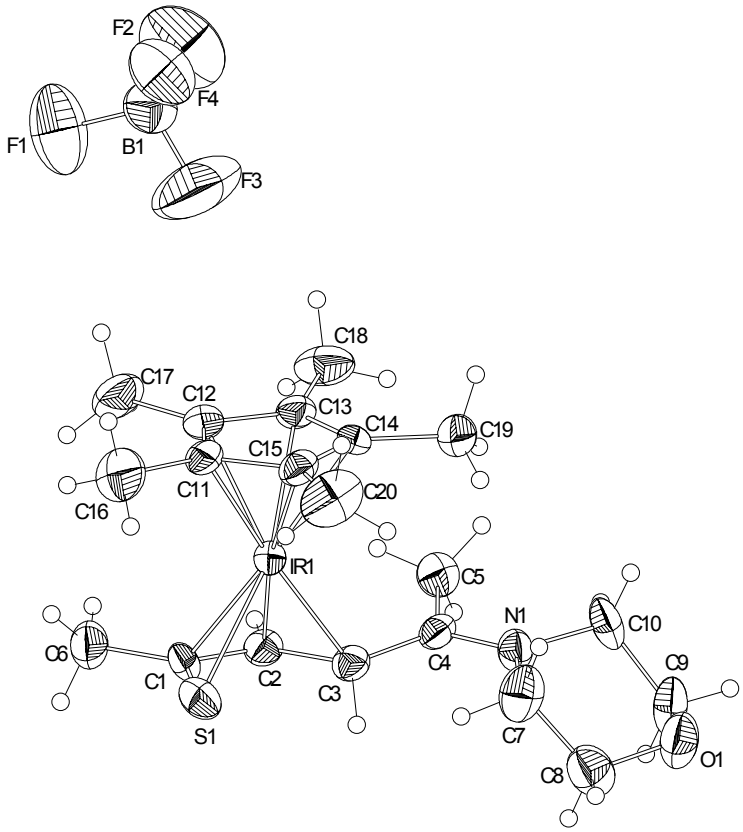

ORTEP drawing of Compound **14**

Formula Minima : C_{20} H_{31} B F_4 Ir N O S

Autores : Marisol Cervantez Vásquez y Ángeles Paz Sandoval

Tab. 1 Crystal data and data collection

Tab. 2 Solution and refinement

Tab. 3 Atomic coordinates and equivalent isotropic displacement parameters

Tab. 4 Bond lengths and angles

Tab. 5 Anisotropic displacement parameters

Tab. 6 Hydrogen coordinates and isotropic displacement parameters

Table 1. Crystal data and data collection compound **14**

Identification code	Compound **14**	
Operator	BPM	
Empirical formula	C_{20} H_{31} B F_4 Ir N O S	
Formula weight	612.53	
Crystal size	0.25 x 0.23 x 0.10 mm	
Crystal color and habit	red prism	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.3432(2) Å	α = 95.8270(10°)
	b = 11.4873(3) Å	β = 108.9380(9°)
	c = 12.5263(4) Å	γ = 97.3639(10°)
Volume	1113.00(5) $Å^3$	
Z	2	
Density (calculated)	1.828 Mg/m^3	
Absorption coefficient	6.136 mm^{-1}	
F(000)	600	
Diffractometer used	Kappa CCD	
Radiation and wavelength	MoKα with λ=0.71073 Å	
Scan type	ω−φ	
Temperature	298(2) K	
2θ range for data collection	5.84 to 55.08°	
Index ranges	$-10 \le h \le 10$ $-12 \le k \le 14$ $-16 \le l \le 14$	
Reflections collected	10670	
Independent reflections	5058 (R_{int} = 0.0729)	
Observed reflections	4204 (F>4σ(F))	
Absorption correction	Multi-scan	
Max. and min. transmission	0.44380 and 0.20185	

Experimental details :

Scan speed	Variable; 16.1 to 60 °/min in ω
Scan range (ω)	0.7 °

Background measurement : Moving crystal and moving counter at the beginning and end of scan, each for 25% of total scan area.

Crystal mounted on a loop.

Table 2. Solution and refinement

Structure solution program	SHELXS-97(Sheldrick 1990)
Solution	heavy-atom-method
Refinement method	Full-matrix Least-Squares on F^2
Extinction correction	SHELXL
Extinction coefficients	0.0038(9)
Hydrogen atoms	constr
Weighting scheme	$w^{-1}=\sigma^2Fo^2+(P)^2+P$ where $P=(Fo^2+2Fc^2)/3$
Data / restraints / parameters	5058 / 0 / 270
Data-to-parameter-ratio	18.7 : 1 (15.6 : 1 [F>4σ(F)])
Final R indices [F>4σ(F)]	R1 = 0.0560, wR2 = 0.1254
R indices (all data)	R1 = 0.0698, wR2 = 0.1313
Goodness-of-Fit on F^2	1.071
Largest and mean Δ/σ	0.001 0.000
Largest difference peak	2.854 eÅ^{-3}
Largest difference hole	-1.367 eÅ^{-3}

Refinement details :

Program used	SHELXL-97 (Sheldrick 1997)
CifRtf version used	2.0

Table 3. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for compound **14.** U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor

	x	y	z	U(eq)
C(1)	10879(10)	8930(7)	8074(7)	35.7(19)
C(2)	9689(10)	9088(7)	8629(7)	32.6(17)
C(3)	9156(10)	8077(7)	9124(7)	31.3(17)
C(4)	7681(10)	7975(7)	9484(7)	30.4(17)
C(5)	6549(12)	8905(8)	9280(8)	45(2)
C(6)	11486(12)	9894(8)	7496(8)	49(2)
C(7)	8153(14)	6025(8)	10054(9)	53(3)
C(8)	8621(12)	5726(9)	11249(10)	55(3)
C(9)	6461(13)	6593(8)	11583(9)	51(2)
C(10)	5832(11)	6930(9)	10396(9)	47(2)
C(11)	7981(11)	6868(8)	5516(7)	36.2(19)
C(12)	7184(10)	7884(7)	5542(7)	34.8(18)
C(13)	5990(10)	7674(7)	6112(7)	33.6(18)
C(14)	6030(9)	6515(7)	6431(7)	31.2(17)
C(15)	7256(11)	5992(7)	6063(7)	33.4(18)
C(16)	9284(14)	6671(10)	4940(9)	61(3)
C(17)	7506(14)	8967(9)	4995(9)	63(3)
C(18)	4725(13)	8482(10)	6190(9)	57(3)
C(19)	4909(12)	5923(9)	7007(8)	52(2)
C(20)	7660(15)	4780(8)	6186(9)	66(3)
B(1)	2886(17)	7942(10)	2102(12)	59(3)
F(1)	4114(12)	8665(7)	1833(9)	116(3)
F(2)	1457(11)	8394(8)	1942(10)	130(4)
F(3)	3635(17)	7776(10)	3185(9)	169(5)
F(4)	2481(9)	6820(6)	1448(7)	86(2)
Ir(1)	8597.5(3)	7601.1(2)	7286.0(2)	26.3(1)
N(1)	7284(9)	7074(6)	9964(6)	34.4(15)
O(1)	7160(9)	5533(6)	11600(6)	55.5(18)
S(1)	11614(3)	7566(2)	8061(2)	44.1(5)

Table 4. Bond lengths [Å] and angles [°] for compound **14**

C(1)-C(2)	1.404(11)	C(1)-C(6)	1.505(11)
C(1)-S(1)	1.755(9)	C(1)-Ir(1)	2.158(8)
C(2)-C(3)	1.457(11)	C(2)-Ir(1)	2.145(7)
C(3)-C(4)	1.436(11)	C(3)-Ir(1)	2.191(8)
C(4)-N(1)	1.308(10)	C(4)-C(5)	1.502(12)
C(7)-N(1)	1.479(11)	C(7)-C(8)	1.507(14)
C(8)-O(1)	1.423(11)	C(9)-O(1)	1.415(11)
C(9)-C(10)	1.517(13)	C(10)-N(1)	1.477(10)
C(11)-C(12)	1.418(12)	C(11)-C(15)	1.449(11)
C(11)-C(16)	1.514(12)	C(11)-Ir(1)	2.158(8)
C(12)-C(13)	1.413(11)	C(12)-C(17)	1.515(12)
C(12)-Ir(1)	2.200(8)	C(13)-C(14)	1.430(11)
C(13)-C(18)	1.512(11)	C(13)-Ir(1)	2.213(8)
C(14)-C(15)	1.423(11)	C(14)-C(19)	1.494(11)
C(14)-Ir(1)	2.201(7)	C(15)-C(20)	1.486(11)
C(15)-Ir(1)	2.191(8)	B(1)-F(2)	1.325(14)
B(1)-F(3)	1.342(16)	B(1)-F(1)	1.385(15)
B(1)-F(4)	1.393(14)	Ir(1)-S(1)	2.393(2)
C(2)-C(1)-C(6)	121.0(8)	C(2)-C(1)-S(1)	117.8(6)
C(6)-C(1)-S(1)	121.2(7)	C(2)-C(1)-Ir(1)	70.4(4)
C(6)-C(1)-Ir(1)	124.9(6)	S(1)-C(1)-Ir(1)	74.6(3)
C(1)-C(2)-C(3)	116.0(7)	C(1)-C(2)-Ir(1)	71.5(5)
C(3)-C(2)-Ir(1)	72.1(4)	C(4)-C(3)-C(2)	123.2(7)
C(4)-C(3)-Ir(1)	115.4(6)	C(2)-C(3)-Ir(1)	68.7(4)
N(1)-C(4)-C(3)	121.3(7)	N(1)-C(4)-C(5)	119.3(7)
C(3)-C(4)-C(5)	119.5(7)	N(1)-C(7)-C(8)	110.5(8)
O(1)-C(8)-C(7)	111.9(8)	O(1)-C(9)-C(10)	112.4(8)
N(1)-C(10)-C(9)	108.8(7)	C(12)-C(11)-C(15)	109.0(7)
C(12)-C(11)-C(16)	126.3(8)	C(15)-C(11)-C(16)	124.5(8)
C(12)-C(11)-Ir(1)	72.6(5)	C(15)-C(11)-Ir(1)	71.7(4)
C(16)-C(11)-Ir(1)	125.2(6)	C(13)-C(12)-C(11)	107.8(7)
C(13)-C(12)-C(17)	126.8(8)	C(11)-C(12)-C(17)	125.4(8)
C(13)-C(12)-Ir(1)	71.8(5)	C(11)-C(12)-Ir(1)	69.4(4)
C(17)-C(12)-Ir(1)	126.6(6)	C(12)-C(13)-C(14)	108.3(7)
C(12)-C(13)-C(18)	124.0(8)	C(14)-C(13)-C(18)	127.2(8)
C(12)-C(13)-Ir(1)	70.8(5)	C(14)-C(13)-Ir(1)	70.7(4)
C(18)-C(13)-Ir(1)	131.2(6)	C(15)-C(14)-C(13)	109.0(7)
C(15)-C(14)-C(19)	125.4(8)	C(13)-C(14)-C(19)	125.6(8)

C(15)-C(14)-Ir(1)	70.7(4)	C(13)-C(14)-Ir(1)	71.5(4)
C(19)-C(14)-Ir(1)	126.1(6)	C(14)-C(15)-C(11)	106.0(7)
C(14)-C(15)-C(20)	126.6(8)	C(11)-C(15)-C(20)	127.4(8)
C(14)-C(15)-Ir(1)	71.5(4)	C(11)-C(15)-Ir(1)	69.3(4)
C(20)-C(15)-Ir(1)	125.2(6)	F(2)-B(1)-F(3)	113.1(13)
F(2)-B(1)-F(1)	112.2(10)	F(3)-B(1)-F(1)	106.3(11)
F(2)-B(1)-F(4)	108.9(10)	F(3)-B(1)-F(4)	105.7(10)
F(1)-B(1)-F(4)	110.5(11)	C(2)-Ir(1)-C(11)	148.8(3)
C(2)-Ir(1)-C(1)	38.1(3)	C(11)-Ir(1)-C(1)	118.0(3)
C(2)-Ir(1)-C(15)	171.6(3)	C(11)-Ir(1)-C(15)	38.9(3)
C(1)-Ir(1)-C(15)	149.3(3)	C(2)-Ir(1)-C(3)	39.3(3)
C(11)-Ir(1)-C(3)	171.6(3)	C(1)-Ir(1)-C(3)	67.8(3)
C(15)-Ir(1)-C(3)	133.2(3)	C(2)-Ir(1)-C(14)	135.8(3)
C(11)-Ir(1)-C(14)	63.5(3)	C(1)-Ir(1)-C(14)	169.9(3)
C(15)-Ir(1)-C(14)	37.8(3)	C(3)-Ir(1)-C(14)	112.0(3)
C(2)-Ir(1)-C(12)	120.0(3)	C(11)-Ir(1)-C(12)	38.0(3)
C(1)-Ir(1)-C(12)	111.2(3)	C(15)-Ir(1)-C(12)	64.2(3)
C(3)-Ir(1)-C(12)	147.9(3)	C(14)-Ir(1)-C(12)	63.1(3)
C(2)-Ir(1)-C(13)	114.7(3)	C(11)-Ir(1)-C(13)	63.1(3)
C(1)-Ir(1)-C(13)	132.7(3)	C(15)-Ir(1)-C(13)	63.6(3)
C(3)-Ir(1)-C(13)	118.3(3)	C(14)-Ir(1)-C(13)	37.8(3)
C(12)-Ir(1)-C(13)	37.4(3)	C(2)-Ir(1)-S(1)	73.2(2)
C(11)-Ir(1)-S(1)	102.3(2)	C(1)-Ir(1)-S(1)	45.0(2)
C(15)-Ir(1)-S(1)	110.8(2)	C(3)-Ir(1)-S(1)	77.4(2)
C(14)-Ir(1)-S(1)	145.1(2)	C(12)-Ir(1)-S(1)	126.1(2)
C(13)-Ir(1)-S(1)	163.3(2)	C(4)-N(1)-C(10)	124.4(7)
C(4)-N(1)-C(7)	123.8(7)	C(10)-N(1)-C(7)	111.6(7)
C(9)-O(1)-C(8)	108.1(7)	C(1)-S(1)-Ir(1)	60.4(3)

Table 5. Anisotropic displacement parameters [$Å^2$ x 10^3]

	U11	U22	U33	U23	U13	U12
C(1)	25(4)	43(5)	36(5)	5(4)	11(4)	-8(3)
C(2)	36(4)	29(4)	25(4)	-2(3)	7(3)	-6(3)
C(3)	31(4)	39(4)	24(4)	3(3)	9(3)	8(3)
C(4)	36(4)	31(4)	22(4)	5(3)	8(3)	4(3)
C(5)	41(5)	51(5)	45(6)	10(4)	17(4)	9(4)
C(6)	50(6)	52(6)	42(6)	7(4)	20(5)	-9(4)
C(7)	70(7)	36(5)	64(7)	21(4)	33(6)	17(5)
C(8)	46(6)	48(6)	74(8)	17(5)	21(5)	8(4)
C(9)	62(6)	49(5)	62(7)	22(5)	43(5)	13(5)
C(10)	33(5)	50(5)	67(7)	13(5)	30(5)	1(4)
C(11)	33(4)	56(5)	19(4)	4(4)	10(3)	5(4)
C(12)	30(4)	41(5)	33(5)	13(4)	6(4)	10(3)
C(13)	27(4)	45(5)	31(5)	13(4)	7(3)	15(3)
C(14)	20(4)	43(5)	24(4)	4(3)	3(3)	-5(3)
C(15)	39(5)	32(4)	24(4)	4(3)	6(4)	2(3)
C(16)	57(7)	91(8)	51(7)	10(6)	34(6)	29(6)
C(17)	70(7)	59(6)	49(7)	30(5)	5(5)	2(5)
C(18)	49(6)	77(7)	42(6)	1(5)	6(5)	31(5)
C(19)	45(6)	64(6)	40(6)	15(5)	9(4)	-12(4)
C(20)	100(9)	28(5)	63(7)	3(4)	18(7)	15(5)
B(1)	59(8)	41(6)	68(9)	9(6)	14(7)	2(6)
F(1)	132(7)	64(5)	175(9)	24(5)	88(7)	-4(4)
F(2)	106(7)	95(6)	199(11)	12(6)	58(7)	51(5)
F(3)	212(12)	141(9)	75(7)	39(6)	-35(7)	-48(8)
F(4)	76(5)	64(4)	111(6)	-9(4)	32(4)	2(3)
Ir(1)	24.9(2)	28.3(2)	26.4(2)	6.9(1)	9.4(1)	3.5(1)
N(1)	33(4)	39(4)	36(4)	9(3)	18(3)	7(3)
O(1)	63(4)	57(4)	65(5)	31(3)	37(4)	17(3)
S(1)	27.4(11)	54.2(14)	51.9(14)	11.0(10)	14.2(10)	7.5(9)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for compound **14**

	x	y	z	U(eq)
H(2)	9175	9808	8628	39
H(3)	10113	7740	9600	38
H(5A)	6821	9446	9975	67
H(5B)	5366	8530	9036	67
H(5C)	6737	9332	8699	67
H(6A)	12608	10302	7975	73
H(6B)	10697	10447	7363	73
H(6C)	11540	9549	6780	73
H(7A)	9185	6188	9859	63
H(7B)	7396	5352	9518	63
H(8A)	9142	5016	11283	66
H(8B)	9462	6370	11773	66
H(9A)	7331	7234	12090	61
H(9B)	5509	6493	11869	61
H(10A)	4915	6316	9890	57
H(10B)	5384	7667	10423	57
H(16A)	10083	6216	5371	92
H(16B)	9895	7425	4903	92
H(16C)	8702	6248	4181	92
H(17A)	8667	9080	4996	94
H(17B)	7332	9655	5419	94
H(17C)	6723	8853	4222	94
H(18A)	5308	9291	6400	86
H(18B)	4239	8275	6757	86
H(18C)	3824	8393	5463	86
H(19A)	4655	6512	7501	78
H(19B)	5494	5372	7450	78
H(19C)	3857	5506	6442	78
H(20A)	7585	4577	6895	99
H(20B)	8803	4760	6178	99
H(20C)	6852	4219	5564	99

Table 7. Crystal data and data collection parameters:

Compound	Compound **14**
Chem. formula	C_{20} H_{31} B F_4 Ir N O S
Form. wght.	612.53
Cryst. size [mm]	0.10x0.23x0.25
Cryst. system	Triclinic
Space group	Triclinic
a, [Å]	8.3432(2)
b, [Å]	11.4873(3)
c, [Å]	12.5263(4)
α, [°]	95.8270(10)
β, [°]	108.9380(9)
γ, [°]	97.3639(10)
V, [Å^3]	1113.00(5)
Z	2
ρ(calcd.), [Mg/m^3]	1.828
μ [mm^{-1}]	6.136
F(000)	600
Index range	-10≤h≤10-12≤k≤14-16≤l≤14
2 θ [°]	55.08
Temp, [K]	298(2)
Refl. collected	10670
Refl. unique	5058
Refl. observed (4σ)	4204
R (int.)	0.0729
No. variables	270
Weighting scheme[1] x/y	/
GOOF	1.071
Final R (4σ)	0.0560
Final wR2	0.1254
Larg. res. peak [e/Å^3]	2.854

[1] $w^{-1} = \sigma^2 F_o^2 + (xP)^2 + yP$; $P = (F_o^2 + 2F_c^2)/3$

Selected torsion angles of compound 14

177.99 (0.74) C6 - C1 - C2 - C3
-1.19 (1.02) S1 - C1 - C2 - C3
58.40 (0.62) Ir1 - C1 - C2 - C3
119.60 (0.79) C6 - C1 - C2 - Ir1
-59.59 (0.52) S1 - C1 - C2 - Ir1
-165.17 (0.75) C1 - C2 - C3 - C4
-107.09 (0.76) Ir1 - C2 - C3 - C4
-58.08 (0.63) C1 - C2 - C3 - Ir1
-177.35 (0.75) C2 - C3 - C4 - N1
102.52 (0.81) Ir1 - C3 - C4 - N1
4.10 (1.19) C2 - C3 - C4 - C5
-76.04 (0.84) Ir1 - C3 - C4 - C5
56.41 (1.07) N1 - C7 - C8 - O1
-58.47 (1.00) O1 - C9 - C10 - N1
1.01 (0.96) C15 - C11 - C12 - C13
176.83 (0.86) C16 - C11 - C12 - C13
-61.92 (0.61) Ir1 - C11 - C12 - C13
-176.08 (0.83) C15 - C11 - C12 - C17
-0.26 (1.45) C16 - C11 - C12 - C17
120.99 (0.88) Ir1 - C11 - C12 - C17
62.93 (0.56) C15 - C11 - C12 - Ir1
-121.25 (0.93) C16 - C11 - C12 - Ir1
-0.69 (0.96) C11 - C12 - C13 - C14
176.35 (0.85) C17 - C12 - C13 - C14
-61.09 (0.56) Ir1 - C12 - C13 - C14
-172.25 (0.80) C11 - C12 - C13 - C18
4.78 (1.43) C17 - C12 - C13 - C18
127.34 (0.86) Ir1 - C12 - C13 - C18
60.40 (0.58) C11 - C12 - C13 - Ir1
-122.56 (0.92) C17 - C12 - C13 - Ir1
0.11 (0.93) C12 - C13 - C14 - C15
171.33 (0.81) C18 - C13 - C14 - C15
-61.09 (0.54) Ir1 - C13 - C14 - C15
-177.19 (0.80) C12 - C13 - C14 - C19
-5.97 (1.40) C18 - C13 - C14 - C19
121.61 (0.84) Ir1 - C13 - C14 - C19
61.20 (0.59) C12 - C13 - C14 - Ir1
-127.58 (0.89) C18 - C13 - C14 - Ir1

0.50 (0.88) C13 - C14 - C15 - C11
177.80 (0.78) C19 - C14 - C15 - C11
-61.12 (0.53) Ir1 - C14 - C15 - C11
-177.80 (0.86) C13 - C14 - C15 - C20
-0.50 (1.37) C19 - C14 - C15 - C20
120.58 (0.90) Ir1 - C14 - C15 - C20
61.62 (0.56) C13 - C14 - C15 - Ir1
-121.08 (0.82) C19 - C14 - C15 - Ir1
-0.93 (0.90) C12 - C11 - C15 - C14
-176.85 (0.83) C16 - C11 - C15 - C14
62.56 (0.53) Ir1 - C11 - C15 - C14
177.35 (0.88) C12 - C11 - C15 - C20
1.43 (1.44) C16 - C11 - C15 - C20
-119.16 (0.91) Ir1 - C11 - C15 - C20
-63.49 (0.58) C12 - C11 - C15 - Ir1
120.59 (0.88) C16 - C11 - C15 - Ir1
-50.15 (0.83) C1 - C2 - Ir1 - C11
-176.55 (0.48) C3 - C2 - Ir1 - C11
-126.40 (0.73) C3 - C2 - Ir1 - C1
154.85 (1.76) C1 - C2 - Ir1 - C15
28.45 (2.09) C3 - C2 - Ir1 - C15
126.40 (0.73) C1 - C2 - Ir1 - C3
-167.71 (0.45) C1 - C2 - Ir1 - C14
65.90 (0.63) C3 - C2 - Ir1 - C14
-86.61 (0.57) C1 - C2 - Ir1 - C12
146.99 (0.46) C3 - C2 - Ir1 - C12
-128.47 (0.51) C1 - C2 - Ir1 - C13
105.13 (0.49) C3 - C2 - Ir1 - C13
35.76 (0.46) C1 - C2 - Ir1 - S1
-90.64 (0.44) C3 - C2 - Ir1 - S1
-56.78 (0.80) C12 - C11 - Ir1 - C2
-174.35 (0.51) C15 - C11 - Ir1 - C2
65.85 (1.07) C16 - C11 - Ir1 - C2
-89.21 (0.54) C12 - C11 - Ir1 - C1
153.21 (0.48) C15 - C11 - Ir1 - C1
33.41 (0.94) C16 - C11 - Ir1 - C1
117.58 (0.69) C12 - C11 - Ir1 - C15
-119.80 (1.02) C16 - C11 - Ir1 - C15
138.42 (1.73) C12 - C11 - Ir1 - C3
20.85 (2.01) C15 - C11 - Ir1 - C3

-98.95 (1.94) C16 - C11 - Ir1 - C3
79.52 (0.52) C12 - C11 - Ir1 - C14
-38.06 (0.46) C15 - C11 - Ir1 - C14
-157.86 (0.93) C16 - C11 - Ir1 - C14
-117.58 (0.69) C15 - C11 - Ir1 - C12
122.62 (1.03) C16 - C11 - Ir1 - C12
37.00 (0.47) C12 - C11 - Ir1 - C13
-80.58 (0.51) C15 - C11 - Ir1 - C13
159.62 (0.94) C16 - C11 - Ir1 - C13
-134.47 (0.45) C12 - C11 - Ir1 - S1
107.96 (0.44) C15 - C11 - Ir1 - S1
-11.84 (0.85) C16 - C11 - Ir1 - S1
-114.75 (0.96) C6 - C1 - Ir1 - C2
127.71 (0.62) S1 - C1 - Ir1 - C2
153.28 (0.49) C2 - C1 - Ir1 - C11
38.52 (0.86) C6 - C1 - Ir1 - C11
-79.01 (0.39) S1 - C1 - Ir1 - C11
-173.00 (0.50) C2 - C1 - Ir1 - C15
72.25 (0.99) C6 - C1 - Ir1 - C15
-45.29 (0.70) S1 - C1 - Ir1 - C15
-33.38 (0.49) C2 - C1 - Ir1 - C3
-148.13 (0.83) C6 - C1 - Ir1 - C3
94.33 (0.35) S1 - C1 - Ir1 - C3
57.67 (1.76) C2 - C1 - Ir1 - C14
-57.08 (1.93) C6 - C1 - Ir1 - C14
-174.62 (1.44) S1 - C1 - Ir1 - C14
112.00 (0.52) C2 - C1 - Ir1 - C12
-2.76 (0.84) C6 - C1 - Ir1 - C12
-120.29 (0.32) S1 - C1 - Ir1 - C12
75.27 (0.62) C2 - C1 - Ir1 - C13
-39.48 (0.93) C6 - C1 - Ir1 - C13
-157.02 (0.33) S1 - C1 - Ir1 - C13
-127.71 (0.62) C2 - C1 - Ir1 - S1
117.54 (0.85) C6 - C1 - Ir1 - S1
43.75 (2.04) C14 - C15 - Ir1 - C2
159.64 (1.79) C11 - C15 - Ir1 - C2
-78.49 (2.15) C20 - C15 - Ir1 - C2
-115.88 (0.66) C14 - C15 - Ir1 - C11
121.87 (1.02) C20 - C15 - Ir1 - C11
-167.19 (0.53) C14 - C15 - Ir1 - C1

-51.31 (0.79) C11 - C15 - Ir1 - C1
70.56 (1.04) C20 - C15 - Ir1 - C1
68.18 (0.59) C14 - C15 - Ir1 - C3
-175.93 (0.40) C11 - C15 - Ir1 - C3
-54.06 (0.97) C20 - C15 - Ir1 - C3
115.88 (0.66) C11 - C15 - Ir1 - C14
-122.25 (1.01) C20 - C15 - Ir1 - C14
-78.63 (0.50) C14 - C15 - Ir1 - C12
37.25 (0.47) C11 - C15 - Ir1 - C12
159.12 (0.92) C20 - C15 - Ir1 - C12
-36.87 (0.46) C14 - C15 - Ir1 - C13
79.01 (0.50) C11 - C15 - Ir1 - C13
-159.12 (0.92) C20 - C15 - Ir1 - C13
160.31 (0.40) C14 - C15 - Ir1 - S1
-83.81 (0.46) C11 - C15 - Ir1 - S1
38.06 (0.86) C20 - C15 - Ir1 - S1
117.70 (0.78) C4 - C3 - Ir1 - C2
-74.67 (1.95) C4 - C3 - Ir1 - C11
167.63 (1.71) C2 - C3 - Ir1 - C11
150.14 (0.67) C4 - C3 - Ir1 - C1
32.44 (0.48) C2 - C3 - Ir1 - C1
-56.81 (0.73) C4 - C3 - Ir1 - C15
-174.52 (0.42) C2 - C3 - Ir1 - C15
-18.94 (0.67) C4 - C3 - Ir1 - C14
-136.64 (0.48) C2 - C3 - Ir1 - C14
55.18 (0.88) C4 - C3 - Ir1 - C12
-62.52 (0.75) C2 - C3 - Ir1 - C12
22.44 (0.69) C4 - C3 - Ir1 - C13
-95.27 (0.52) C2 - C3 - Ir1 - C13
-163.62 (0.61) C4 - C3 - Ir1 - S1
78.67 (0.44) C2 - C3 - Ir1 - S1
-171.66 (0.43) C15 - C14 - Ir1 - C2
69.66 (0.62) C13 - C14 - Ir1 - C2
-51.37 (0.93) C19 - C14 - Ir1 - C2
39.17 (0.46) C15 - C14 - Ir1 - C11
-79.51 (0.52) C13 - C14 - Ir1 - C11
159.47 (0.88) C19 - C14 - Ir1 - C11
139.95 (1.52) C15 - C14 - Ir1 - C1
21.27 (1.79) C13 - C14 - Ir1 - C1
-99.76 (1.68) C19 - C14 - Ir1 - C1

-118.68 (0.68) C13 - C14 - Ir1 - C15
120.29 (0.96) C19 - C14 - Ir1 - C15
-133.12 (0.47) C15 - C14 - Ir1 - C3
108.20 (0.49) C13 - C14 - Ir1 - C3
-12.83 (0.85) C19 - C14 - Ir1 - C3
81.86 (0.51) C15 - C14 - Ir1 - C12
-36.82 (0.46) C13 - C14 - Ir1 - C12
-157.85 (0.88) C19 - C14 - Ir1 - C12
118.68 (0.68) C15 - C14 - Ir1 - C13
-121.03 (0.97) C19 - C14 - Ir1 - C13
-33.39 (0.66) C15 - C14 - Ir1 - S1
-152.07 (0.40) C13 - C14 - Ir1 - S1
86.90 (0.84) C19 - C14 - Ir1 - S1
-92.17 (0.54) C13 - C12 - Ir1 - C2
150.01 (0.49) C11 - C12 - Ir1 - C2
30.57 (0.92) C17 - C12 - Ir1 - C2
117.82 (0.71) C13 - C12 - Ir1 - C11
-119.44 (1.02) C17 - C12 - Ir1 - C11
-133.54 (0.50) C13 - C12 - Ir1 - C1
108.64 (0.52) C11 - C12 - Ir1 - C1
-10.80 (0.91) C17 - C12 - Ir1 - C1
79.62 (0.52) C13 - C12 - Ir1 - C15
-38.19 (0.48) C11 - C12 - Ir1 - C15
-157.64 (0.92) C17 - C12 - Ir1 - C15
-51.74 (0.78) C13 - C12 - Ir1 - C3
-169.56 (0.51) C11 - C12 - Ir1 - C3
71.00 (1.04) C17 - C12 - Ir1 - C3
37.25 (0.47) C13 - C12 - Ir1 - C14
-80.57 (0.53) C11 - C12 - Ir1 - C14
159.99 (0.93) C17 - C12 - Ir1 - C14
-117.82 (0.71) C11 - C12 - Ir1 - C13
122.74 (1.02) C17 - C12 - Ir1 - C13
177.43 (0.38) C13 - C12 - Ir1 - S1
59.61 (0.54) C11 - C12 - Ir1 - S1
-59.83 (0.88) C17 - C12 - Ir1 - S1
107.79 (0.51) C12 - C13 - Ir1 - C2
-133.97 (0.48) C14 - C13 - Ir1 - C2
-11.04 (0.95) C18 - C13 - Ir1 - C2
-37.59 (0.49) C12 - C13 - Ir1 - C11
80.65 (0.52) C14 - C13 - Ir1 - C11

-156.42 (0.96) C18 - C13 - Ir1 - C11
66.73 (0.63) C12 - C13 - Ir1 - C1
-175.03 (0.43) C14 - C13 - Ir1 - C1
-52.10 (0.99) C18 - C13 - Ir1 - C1
-81.35 (0.52) C12 - C13 - Ir1 - C15
36.89 (0.47) C14 - C13 - Ir1 - C15
159.82 (0.95) C18 - C13 - Ir1 - C15
151.71 (0.47) C12 - C13 - Ir1 - C3
-90.05 (0.52) C14 - C13 - Ir1 - C3
32.88 (0.94) C18 - C13 - Ir1 - C3
-118.24 (0.69) C12 - C13 - Ir1 - C14
122.93 (1.04) C18 - C13 - Ir1 - C14
118.24 (0.69) C14 - C13 - Ir1 - C12
-118.83 (1.04) C18 - C13 - Ir1 - C12
-7.26 (1.07) C12 - C13 - Ir1 - S1
110.98 (0.78) C14 - C13 - Ir1 - S1
-126.09 (0.86) C18 - C13 - Ir1 - S1
177.55 (0.79) C3 - C4 - N1 - C10
-3.89 (1.28) C5 - C4 - N1 - C10
-7.72 (1.28) C3 - C4 - N1 - C7
170.85 (0.83) C5 - C4 - N1 - C7
-132.73 (0.87) C9 - C10 - N1 - C4
51.97 (1.00) C9 - C10 - N1 - C7
132.89 (0.88) C8 - C7 - N1 - C4
-51.78 (1.06) C8 - C7 - N1 - C10
62.55 (1.06) C10 - C9 - O1 - C8
-61.00 (1.05) C7 - C8 - O1 - C9
57.43 (0.58) C2 - C1 - S1 - Ir1
-121.75 (0.78) C6 - C1 - S1 - Ir1
-30.67 (0.40) C2 - Ir1 - S1 - C1
117.46 (0.41) C11 - Ir1 - S1 - C1
157.19 (0.40) C15 - Ir1 - S1 - C1
-71.08 (0.39) C3 - Ir1 - S1 - C1
178.35 (0.44) C14 - Ir1 - S1 - C1
84.58 (0.43) C12 - Ir1 - S1 - C1
90.02 (0.83) C13 - Ir1 - S1 - C1