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Experimental Procedure

Crystallographic Structural Determination. Two samples of crystals were received for analysis. One sample consisted of matted clumps of well formed crystals, and the other, large, separated and fully faceted. The data specimen was cleaved from a large crystal from the second sample. Both samples appeared by microscopy to be of a single morphology. Crystal, data collection, and refinement parameters for [(hfac)Ir(1,5-COD)] (**1**) (hfac: hexafluoroacetylacetonato; 1,5-COD: 1,5-cyclooctadiene) are given in Table I. The data crystal was mounted on a glass fiber. The data were collected on a Siemens P4 diffractometer equipped with a SMART CCD detector. A dark red, block-shaped crystal was found to belong to the orthorhombic crystal system. The systematic absences in the diffraction data indicated that the space group could be uniquely assigned as *Pbca*. Semi-empirical corrections for absorption were applied to the data. The structure was solved using direct methods, completed by subsequent difference Fourier syntheses and refined by full-matrix, least-squares procedures. All non-hydrogen atoms were refined with anisotropic displacement coefficients. All hydrogen atoms were treated as idealized contributions. The highest peak on the final difference map of **1**, 0.91 e/Å^3, was in a chemically unreasonable position, 1.06 Å from the metal, and was considered noise. Tables of atomic coordinates, bond distances and angles, anisotropic thermal parameters, and calculated hydrogen atom coordinates follow. All software and sources of the scattering factors are contained in the SHELXTL (version 5.03) program library (G. Sheldrick, Siemens XRD, Madison, WI).

Structure Description

There are two identical, but crystallographically independent, molecules in the asymmetric unit as shown in Figure 1. The bond lengths and angles are given in Table 3. Fluorine atoms in one of trifluoromethyl groups of each molecule were disordered between two positions as follows: F(1)/F(1A), F(2)/F(2A), and F(3)/F(3A) in a 60:40 ratio; F(4')/F(4'A), F(5')/F(5'A), and F(6')/F(6'A) in a 44:56 ratio(see Figures 1 and 2). The packing diagram (Figure 3) shows that these disordered fluorine atoms are closely packed and occupy mutually exclusive rotational positions. This is very clearly seen in the space-filling diagram (Figure 4). Each molecule has a nearly perfectly square planar geometry around iridium metal (based on the C=C centroids). The maximum deviation from planarity is *ca.* 0.02 Å and the angles are within 2 ° of 90 or 180 °. The average bond distance of Ir-O is 2.07 Å, which matches well with that of related iridium complexes (average d(Ir-O) 2.08 Å).[1]

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(1) From Cambridge Database

Table I. Crystal, Data Collection, and Refinement Parameters for [(hfac)Ir(1,5-COD)] (**1**).

	1
Empirical formula	$C_{13}H_{13}F_6IrO_4$
Fw	507.43
Cryst syst	Orthorhombic
Space group	*Pbca*
a, Å	17.6226(2)
b, Å	16.3050(3)
c, Å	20.3016(3)
V, Å^3	5833.4(2)
Z	16
ρ_{calc} g/cm^3	2.311
Cryst color and habit	dark red block
Abs coeff, mm^{-1}	9.225
Temp, K	198(2)
2θ scan range, deg	4.0 - 56.7
No. of rflns collected	22300
No. of indep rflns	6824
Transmission(min, max)	0.745, 0.888
N_o/N_v	15.0
GOF	1.074
R(*F*), %[a]	2.79
$R_w(F^2)$, %[a]	7.35
Diff peak (min, max) e/Å^3	0.914, -0.878

[a] Quantity minimized = $R(F) = \sum||F_o| - |F_c||/\sum|F_o|$; $R_w(F^2) = [\sum[w(F_o^2 - F_c^2)^2]/\sum[(wF_o^2)^2]]^{1/2}$.

Figure Captions

Figure 1. Molecular Structure of **1** drawn with 30 % thermal ellipsoids. Hydrogen atoms are omitted for clarity. It shows two identical, but crystallographically independent molecules in the asymmetric unit.

Figure 2. Molecular Structure of **1** showing disordered fluorine atoms.

Figure 3. Packing Diagram of **1**.

Figure 4. Space-filling Diagram of four molecules of **1** with the disordered CF_3 groups speckled.

Figure 1

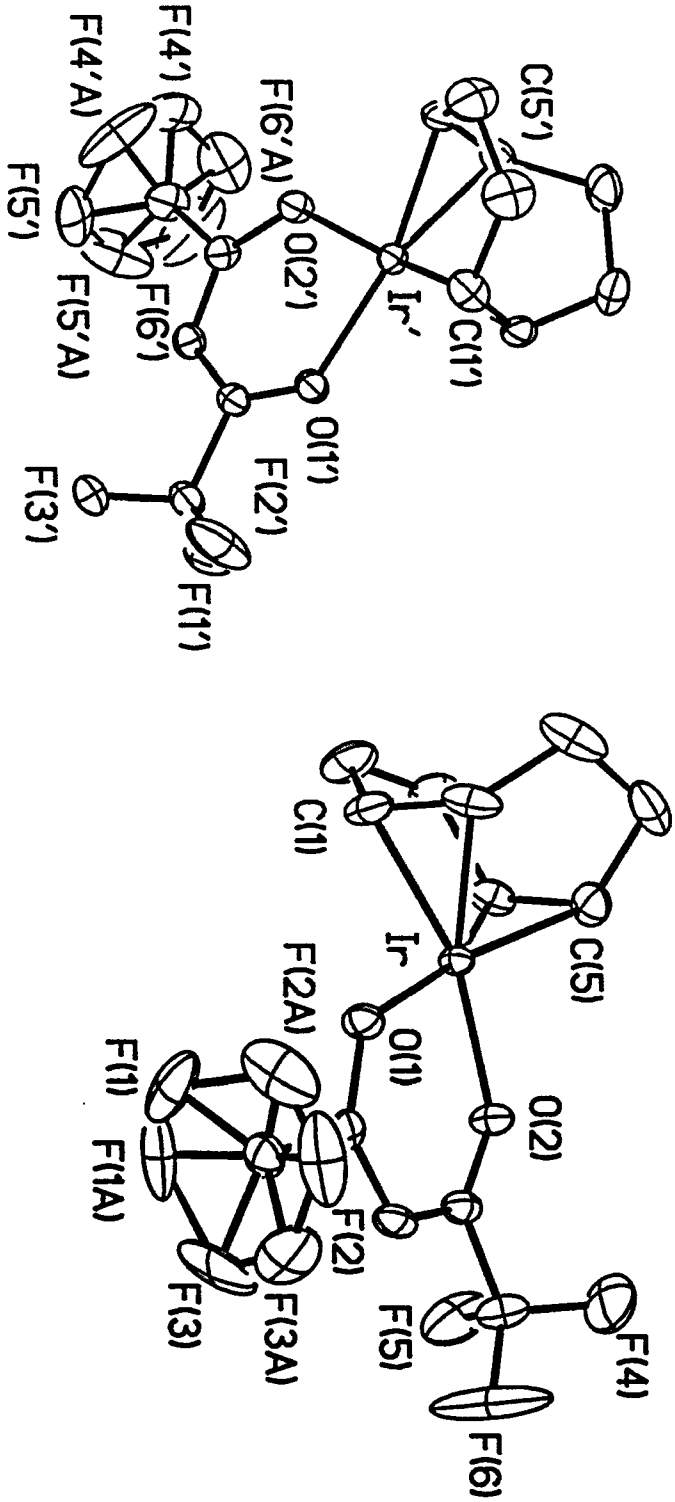

C(5')
F(4')
F(4'A)
F(6'A)
O(2')
F(5')
F(6')
Ir'
C(1')
F(5'A)
O(1')
F(2')
F(3')
F(1')
C(1)
C(5)
Ir
F(2A)
O(1)
O(2)
F(1)
F(1A)
F(2)
F(3)
F(3A)
F(5)
F(4)
F(6)

Figure 2

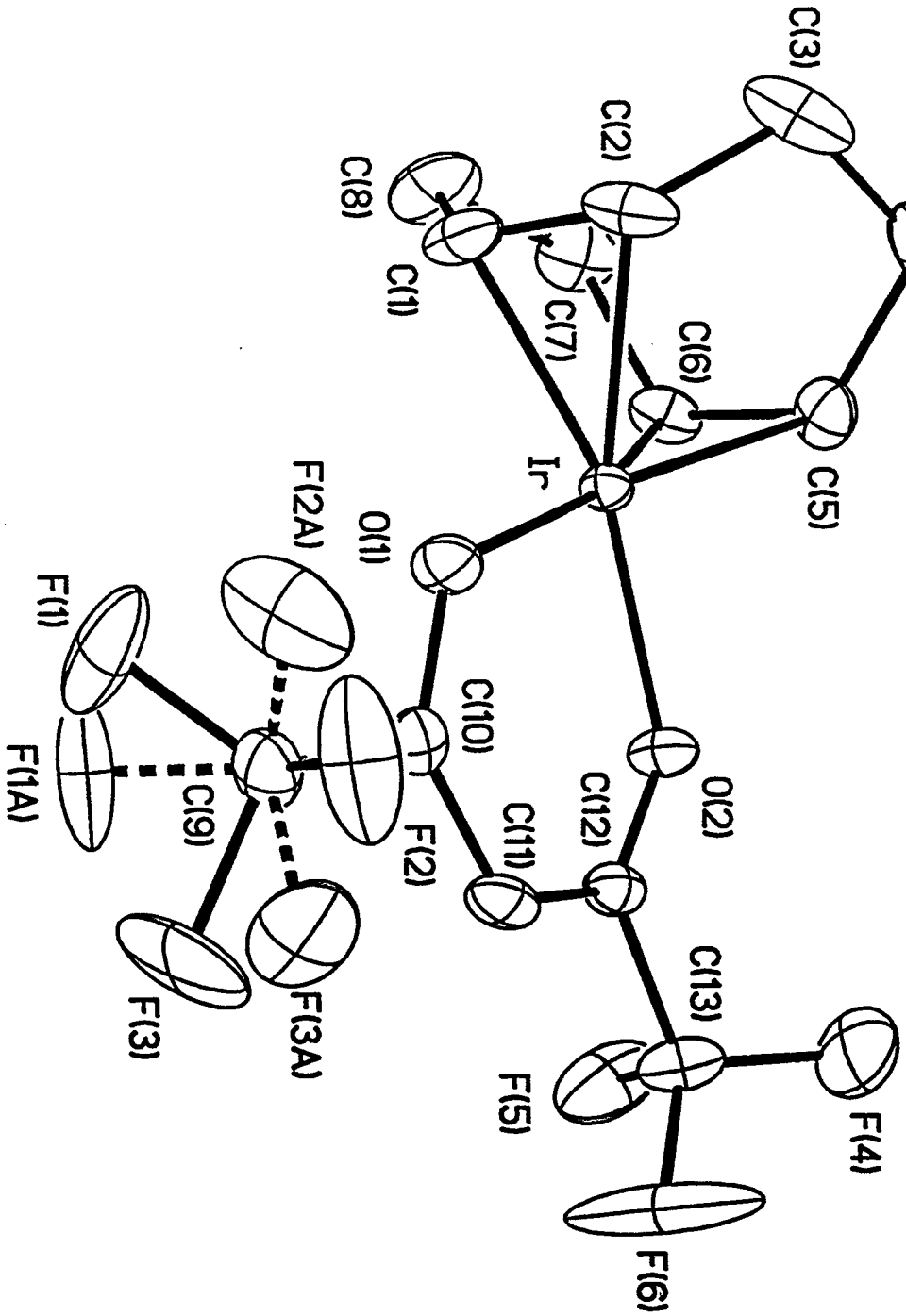

C(3)
C(2)
C(4)
C(8)
C(1)
C(7)
C(6)
Ir
C(5)
F(2A)
O(1)
F(1)
C(10)
O(2)
F(1A)
C(9)
C(11)
C(12)
F(2)
C(13)
F(3)
F(3A)
F(5)
F(4)
F(6)

Figure 3

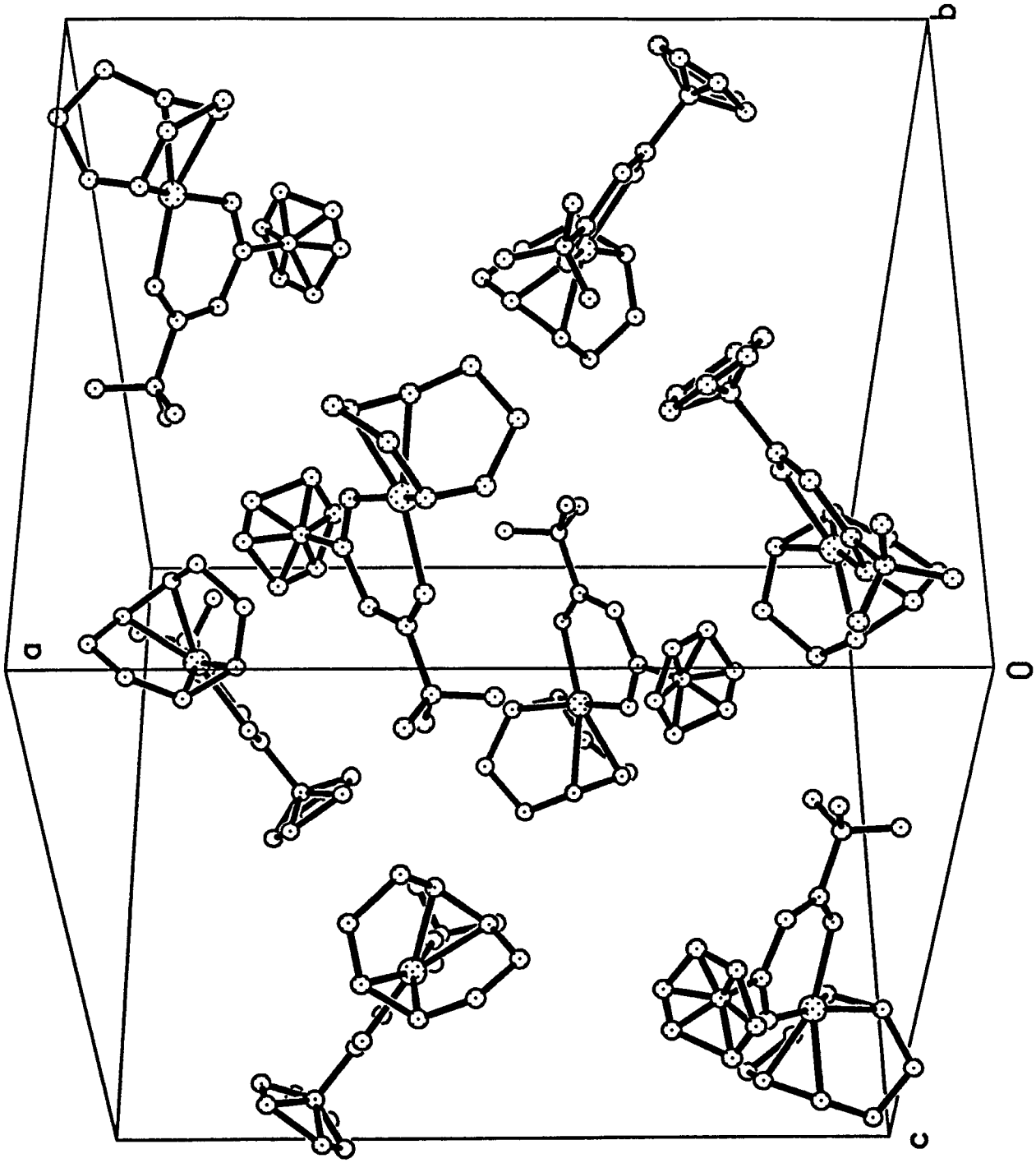


Figure 4

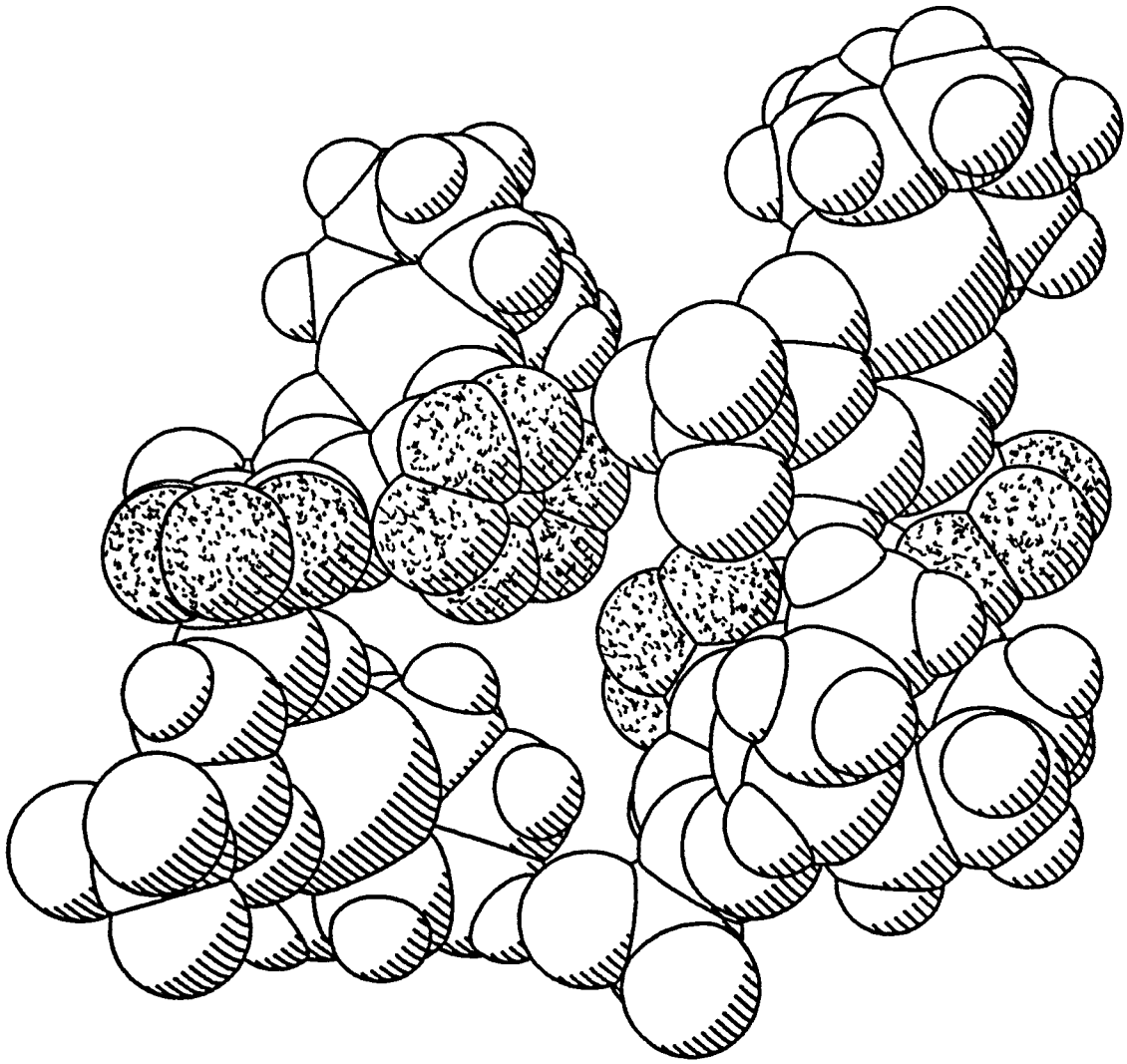


Table 1. Crystal data and structure refinement for 1.

Identification code	atm16
Empirical formula	$C_{13}H_{13}F_6IrO_2$
Formula weight	507.43
Temperature	198(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 17.6226(2) Å alpha = 90° b = 16.3050(3) Å beta = 90° c = 20.3016(3) Å gamma = 90°
Volume, Z	5833.4(2) $Å^3$, 16
Density (calculated)	2.311 g/cm^3
Absorption coefficient	9.225 mm^{-1}
F(000)	3808
Crystal size	0.40 x 0.30 x 0.20 mm
θ range for data collection	1.98 to 28.35°
Limiting indices	$-21 \le h \le 23$, $-19 \le k \le 21$, $-22 \le l \le 25$
Reflections collected	22300
Independent reflections	6824 (R_{int} = 0.0295)
Absorption correction	SADABS
Max. and min. transmission	0.888 and 0.745
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6821 / 0 / 454
Goodness-of-fit on F^2	1.074
Final R indices [I>2σ(I)]	R1 = 0.0279, wR2 = 0.0735
R indices (all data)	R1 = 0.0370, wR2 = 0.0811
Extinction coefficient	0.00012(3)
Largest diff. peak and hole	0.914 and -0.878 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ir	1100.9(1)	4226.2(1)	2968.2(1)	25(1)
F(1)	2922(8)	5403(12)	1596(5)	90(7)
F(1A)	3019(9)	4941(17)	1369(15)	109(10)
F(2)	1990(5)	5723(10)	1001(10)	89(8)
F(2A)	2243(16)	5918(8)	1441(12)	89(10)
F(3)	2650(12)	4745(7)	749(7)	96(7)
F(3A)	2206(13)	5110(18)	677(7)	91(10)
F(4)	66(3)	2437(4)	1421(3)	123(2)
F(5)	1099(3)	1895(2)	1533(2)	86(2)
F(6)	896(5)	2618(3)	703(2)	154(3)
O(1)	1730(2)	4836(2)	2264(2)	34(1)
O(2)	860(2)	3301(2)	2304(2)	34(1)
C(1)	1680(4)	4893(4)	3696(2)	44(1)
C(2)	1008(4)	5301(3)	3534(3)	49(2)
C(3)	318(5)	5293(4)	3991(4)	74(2)
C(4)	-213(4)	4615(5)	3843(3)	61(2)
C(5)	159(3)	3881(4)	3529(3)	43(1)
C(6)	814(3)	3481(3)	3779(2)	38(1)
C(7)	1203(4)	3729(4)	4415(3)	54(2)
C(8)	1809(5)	4380(5)	4307(3)	63(2)
C(9)	2354(3)	5137(4)	1277(2)	43(1)
C(10)	1835(3)	4574(3)	1681(2)	30(1)
C(11)	1533(3)	3880(3)	1382(2)	34(1)
C(12)	1082(3)	3306(3)	1709(2)	33(1)
C(13)	800(4)	2556(3)	1322(2)	46(1)
Ir'	1450(1)	3806(1)	8744(1)	28(1)
F(1')	2791(3)	2670(4)	7013(2)	108(2)
F(2')	2891(3)	1592(2)	7558(2)	83(1)
F(3')	3791(2)	2445(3)	7568(2)	72(1)
F(4')	3192(13)	3368(16)	10445(9)	91(10)
F(4'A)	3621(18)	3453(12)	10161(12)	144(14)
F(5')	3987(6)	2786(19)	9871(7)	81(8)
F(5'A)	3684(17)	2209(16)	9928(6)	130(13)
F(6')	3080(19)	2114(15)	10216(14)	128(17)
F(6'A)	2794(7)	2664(18)	10476(5)	105(8)
O(1')	2074(2)	3177(2)	8041(2)	36(1)
O(2')	2199(2)	3445(2)	9476(2)	37(1)
C(1')	900(4)	4475(4)	7996(2)	47(1)
C(2')	494(3)	3766(4)	8125(3)	44(1)
C(3')	-238(4)	3719(5)	8508(4)	66(2)
C(4')	-186(4)	4069(5)	9192(3)	66(2)
C(5')	628(3)	4117(4)	9453(3)	44(1)
C(6')	1089(3)	4796(3)	9324(3)	41(1)
C(7')	879(5)	5533(4)	8913(4)	66(2)
C(8')	620(5)	5313(4)	8234(3)	64(2)
C(9')	3048(3)	2385(4)	7566(3)	46(1)
C(10')	2681(3)	2806(3)	8172(2)	33(1)
C(11')	3043(3)	2698(3)	8767(2)	38(1)

C(12′)	2783(3)	3010(3)	9364(2)	37(1)
C(13′)	3241(4)	2817(4)	9987(3)	58(2)

Table 3. Bond lengths [Å] and angles [°] for 1.

Ir-O(1)	2.064(3)	Ir-O(2)	2.067(3)
Ir-C(5)	2.090(5)	Ir-C(1)	2.100(5)
Ir-C(2)	2.102(5)	Ir-C(6)	2.108(5)
F(1)-F(1A)	0.90(2)	F(1)-C(9)	1.270(10)
F(1)-F(2A)	1.50(2)	F(1A)-C(9)	1.23(2)
F(1A)-F(3)	1.45(3)	F(2)-F(2A)	1.05(2)
F(2)-F(3A)	1.26(2)	F(2)-C(9)	1.280(9)
F(2A)-C(9)	1.331(13)	F(3)-F(3A)	0.99(2)
F(3)-C(9)	1.353(9)	F(3A)-C(9)	1.246(13)
F(4)-C(13)	1.323(8)	F(5)-C(13)	1.273(7)
F(6)-C(13)	1.272(6)	O(1)-C(10)	1.271(5)
O(2)-C(12)	1.270(6)	C(1)-C(2)	1.397(9)
C(1)-C(8)	1.513(8)	C(2)-C(3)	1.530(9)
C(3)-C(4)	1.479(11)	C(4)-C(5)	1.506(9)
C(5)-C(6)	1.420(8)	C(6)-C(7)	1.515(8)
C(7)-C(8)	1.522(10)	C(9)-C(10)	1.533(7)
C(10)-C(11)	1.390(7)	C(11)-C(12)	1.395(7)
C(12)-C(13)	1.537(7)	Ir'-O(2')	2.072(3)
Ir'-O(1')	2.072(3)	Ir'-C(6')	2.096(5)
Ir'-C(2')	2.103(5)	Ir'-C(5')	2.105(5)
Ir'-C(1')	2.106(5)	F(1')-C(9')	1.296(7)
F(2')-C(9')	1.321(7)	F(3')-C(9')	1.313(6)
F(4')-F(4'A)	0.96(2)	F(4')-C(13')	1.29(2)
F(4')-F(6'A)	1.35(2)	F(4'A)-C(13')	1.28(2)
F(4'A)-F(5')	1.39(2)	F(5')-F(5'A)	1.09(2)
F(5')-C(13')	1.337(14)	F(5'A)-F(6')	1.22(2)
F(5'A)-C(13')	1.268(11)	F(6')-F(6'A)	1.16(3)
F(6')-C(13')	1.269(14)	F(6'A)-C(13')	1.292(13)
O(1')-C(10')	1.258(6)	O(2')-C(12')	1.270(6)
C(1')-C(2')	1.384(9)	C(1')-C(8')	1.532(9)
C(2')-C(3')	1.509(9)	C(3')-C(4')	1.505(10)
C(4')-C(5')	1.530(9)	C(5')-C(6')	1.399(8)
C(6')-C(7')	1.508(8)	C(7')-C(8')	1.497(10)
C(9')-C(10')	1.550(7)	C(10')-C(11')	1.378(7)
C(11')-C(12')	1.392(7)	C(12')-C(13')	1.534(7)

O(1)-Ir-O(2)	90.58(13)	O(1)-Ir-C(5)	159.0(2)
O(2)-Ir-C(5)	89.8(2)	O(1)-Ir-C(1)	88.7(2)
O(2)-Ir-C(1)	159.5(2)	C(5)-Ir-C(1)	98.1(2)
O(1)-Ir-C(2)	91.0(2)	O(2)-Ir-C(2)	161.6(2)
C(5)-Ir-C(2)	82.3(2)	C(1)-Ir-C(2)	38.8(3)
O(1)-Ir-C(6)	161.3(2)	O(2)-Ir-C(6)	92.3(2)
C(5)-Ir-C(6)	39.5(2)	C(1)-Ir-C(6)	82.2(2)
C(2)-Ir-C(6)	92.0(2)	F(1A)-F(1)-C(9)	66.5(14)
F(1A)-F(1)-F(2A)	121(2)	C(9)-F(1)-F(2A)	56.8(7)
F(1)-F(1A)-C(9)	71(2)	F(1)-F(1A)-F(3)	123(2)
C(9)-F(1A)-F(3)	59.9(10)	F(2A)-F(2)-F(3A)	124(2)
F(2A)-F(2)-C(9)	68.9(10)	F(3A)-F(2)-C(9)	58.9(8)
F(2)-F(2A)-C(9)	63.8(9)	F(2)-F(2A)-F(1)	110.4(13)
C(9)-F(2A)-F(1)	53.0(8)	F(3A)-F(3)-C(9)	62.0(9)
F(3A)-F(3)-F(1A)	110.4(14)	C(9)-F(3)-F(1A)	51.9(8)
F(3)-F(3A)-C(9)	73.4(12)	F(3)-F(3A)-F(2)	130(2)
C(9)-F(3A)-F(2)	61.5(9)	C(10)-O(1)-Ir	124.1(3)
C(12)-O(2)-Ir	123.6(3)	C(2)-C(1)-C(8)	125.8(6)
C(2)-C(1)-Ir	70.7(3)	C(8)-C(1)-Ir	111.3(4)

C(1)-C(2)-C(3)	121.7(5)	C(1)-C(2)-Ir	70.5(3)
C(3)-C(2)-Ir	112.7(4)	C(4)-C(3)-C(2)	112.7(5)
C(3)-C(4)-C(5)	113.9(5)	C(6)-C(5)-C(4)	124.6(5)
C(6)-C(5)-Ir	70.9(3)	C(4)-C(5)-Ir	111.2(4)
C(5)-C(6)-C(7)	123.3(5)	C(5)-C(6)-Ir	69.5(3)
C(7)-C(6)-Ir	113.7(4)	C(8)-C(7)-C(6)	112.4(5)
C(7)-C(8)-C(1)	113.4(5)	F(1A)-C(9)-F(3A)	109.7(14)
F(1A)-C(9)-F(1)	42.2(11)	F(3A)-C(9)-F(1)	132.4(9)
F(1A)-C(9)-F(2)	137.5(11)	F(3A)-C(9)-F(2)	59.6(11)
F(1)-C(9)-F(2)	111.3(9)	F(1A)-C(9)-F(2A)	110.5(13)
F(3A)-C(9)-F(2A)	104.3(13)	F(1)-C(9)-F(2A)	70.2(11)
F(2)-C(9)-F(2A)	47.3(9)	F(1A)-C(9)-F(3)	68.3(12)
F(3A)-C(9)-F(3)	44.7(10)	F(1)-C(9)-F(3)	105.1(9)
F(2)-C(9)-F(3)	101.4(9)	F(2A)-C(9)-F(3)	134.9(8)
F(1A)-C(9)-C(10)	109.4(10)	F(3A)-C(9)-C(10)	112.2(8)
F(1)-C(9)-C(10)	113.7(5)	F(2)-C(9)-C(10)	112.5(5)
F(2A)-C(9)-C(10)	110.5(6)	F(3)-C(9)-C(10)	111.9(6)
O(1)-C(10)-C(11)	128.6(4)	O(1)-C(10)-C(9)	112.6(4)
C(11)-C(10)-C(9)	118.8(4)	C(10)-C(11)-C(12)	123.8(4)
O(2)-C(12)-C(11)	129.2(4)	O(2)-C(12)-C(13)	112.4(4)
C(11)-C(12)-C(13)	118.4(4)	F(5)-C(13)-F(6)	110.1(6)
F(5)-C(13)-F(4)	103.3(6)	F(6)-C(13)-F(4)	106.9(6)
F(5)-C(13)-C(12)	111.7(5)	F(6)-C(13)-C(12)	113.5(5)
F(4)-C(13)-C(12)	110.8(5)	O(2')-Ir'-O(1')	90.87(13)
O(2')-Ir'-C(6')	90.5(2)	O(1')-Ir'-C(6')	158.2(2)
O(2')-Ir'-C(2')	158.4(2)	O(1')-Ir'-C(2')	89.9(2)
C(6')-Ir'-C(2')	96.7(2)	O(2')-Ir'-C(5')	90.9(2)
O(1')-Ir'-C(5')	162.7(2)	C(6')-Ir'-C(5')	38.9(2)
C(2')-Ir'-C(5')	82.2(2)	O(2')-Ir'-C(1')	163.2(2)
O(1')-Ir'-C(1')	90.2(2)	C(6')-Ir'-C(1')	82.3(2)
C(2')-Ir'-C(1')	38.4(3)	C(5')-Ir'-C(1')	93.0(2)
F(4'A)-F(4')-C(13')	68(2)	F(4'A)-F(4')-F(6'A)	124(2)
C(13')-F(4')-F(6'A)	58.5(10)	F(4')-F(4'A)-C(13')	69(2)
F(4')-F(4'A)-F(5')	120(2)	C(13')-F(4'A)-F(5')	59.7(10)
F(5'A)-F(5')-C(13')	62.0(10)	F(5'A)-F(5')-F(4'A)	114(2)
C(13')-F(5')-F(4'A)	56.0(9)	F(5')-F(5'A)-F(6')	126(2)
F(5')-F(5'A)-C(13')	68.6(10)	F(6')-F(5'A)-C(13')	61.2(10)
F(6'A)-F(6')-F(5'A)	120(2)	F(6'A)-F(6')-C(13')	64.2(11)
F(5'A)-F(6')-C(13')	61.1(9)	F(6')-F(6'A)-C(13')	62.1(10)
F(6')-F(6'A)-F(4')	114(2)	C(13')-F(6'A)-F(4')	58.7(9)
C(10')-O(1')-Ir'	123.0(3)	C(12')-O(2')-Ir'	123.1(3)
C(2')-C(1')-C(8')	121.3(6)	C(2')-C(1')-Ir'	70.7(3)
C(8')-C(1')-Ir'	112.5(4)	C(1')-C(2')-C(3')	125.6(6)
C(1')-C(2')-Ir'	70.9(3)	C(3')-C(2')-Ir'	112.2(4)
C(4')-C(3')-C(2')	113.8(5)	C(3')-C(4')-C(5')	113.4(5)
C(6')-C(5')-C(4')	121.4(5)	C(6')-C(5')-Ir'	70.2(3)
C(4')-C(5')-Ir'	113.3(4)	C(5')-C(6')-C(7')	126.3(6)
C(5')-C(6')-Ir'	70.9(3)	C(7')-C(6')-Ir'	112.2(4)
C(8')-C(7')-C(6')	113.2(5)	C(7')-C(8')-C(1')	113.9(5)
F(1')-C(9')-F(3')	109.0(5)	F(1')-C(9')-F(2')	105.5(6)
F(3')-C(9')-F(2')	106.3(5)	F(1')-C(9')-C(10')	112.5(5)
F(3')-C(9')-C(10')	112.3(5)	F(2')-C(9')-C(10')	110.8(5)
O(1')-C(10')-C(11')	129.8(5)	O(1')-C(10')-C(9')	113.6(4)
C(11')-C(10')-C(9')	116.6(4)	C(12')-C(11')-C(10')	124.4(5)
O(2')-C(12')-C(11')	128.8(4)	O(2')-C(12')-C(13')	113.2(5)
C(11')-C(12')-C(13')	118.0(5)	F(5'A)-C(13')-F(4'A)	109.7(14)

F(5'A)-C(13')-F(6')	57.7(12)	F(4'A)-C(13')-F(6')	138.3(10)
F(5'A)-C(13')-F(6'A)	107.3(11)	F(4'A)-C(13')-F(6'A)	105.3(12)
F(6')-C(13')-F(6'A)	53.7(13)	F(5'A)-C(13')-F(4')	130.7(11)
F(4'A)-C(13')-F(4')	43.8(11)	F(6')-C(13')-F(4')	110(2)
F(6'A)-C(13')-F(4')	62.7(10)	F(5'A)-C(13')-F(5')	49.4(10)
F(4'A)-C(13')-F(5')	64.3(12)	F(6')-C(13')-F(5')	104.6(14)
F(6'A)-C(13')-F(5')	136.7(8)	F(4')-C(13')-F(5')	102.6(12)
F(5'A)-C(13')-C(12')	114.0(7)	F(4'A)-C(13')-C(12')	109.6(8)
F(6')-C(13')-C(12')	111.6(8)	F(6'A)-C(13')-C(12')	110.6(7)
F(4')-C(13')-C(12')	114.5(8)	F(5')-C(13')-C(12')	112.4(7)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

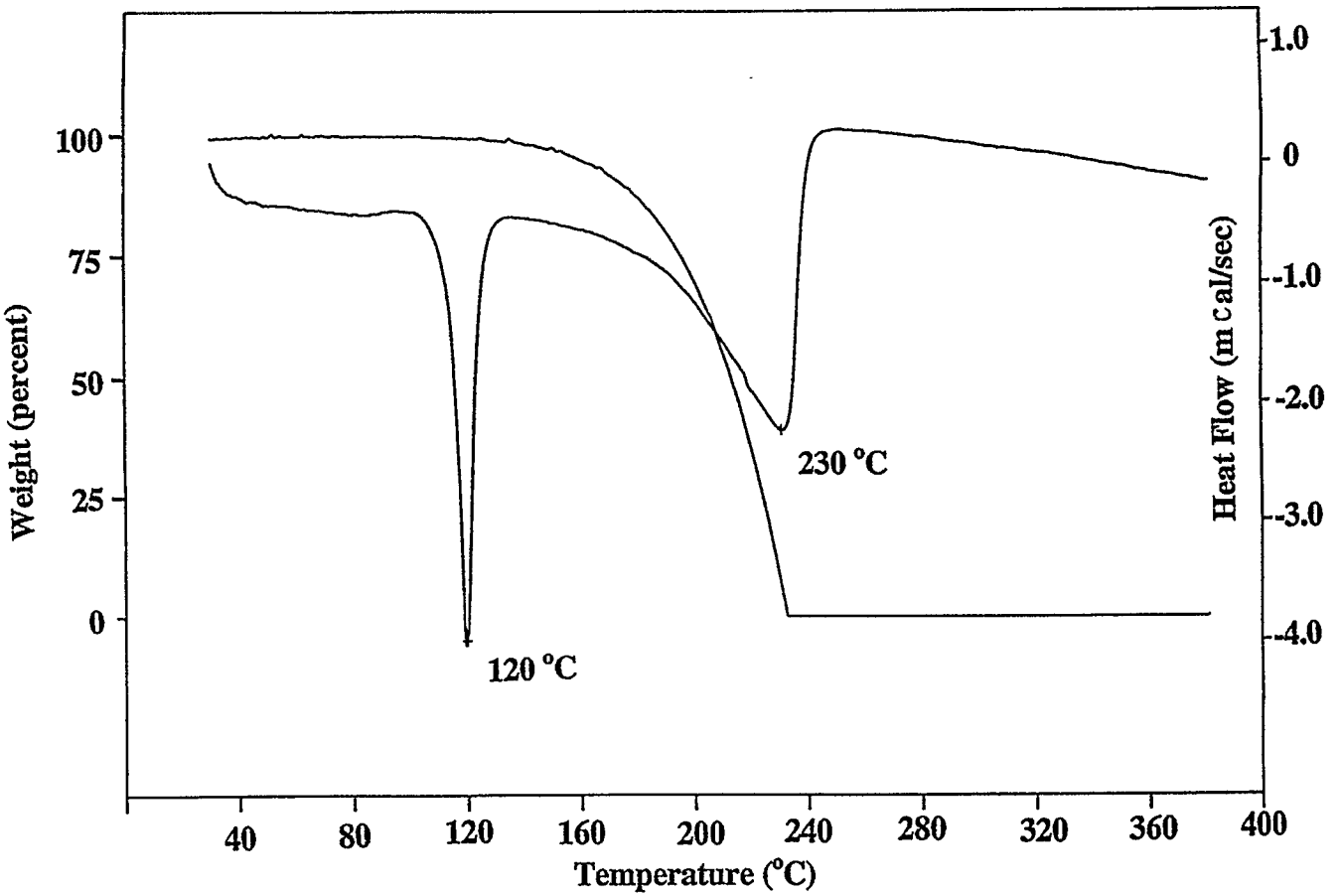
$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ir	29(1)	27(1)	19(1)	-1(1)	1(1)	-2(1)
F(1)	62(8)	160(15)	47(5)	38(6)	-16(4)	-72(10)
F(1A)	23(6)	141(19)	164(24)	34(17)	17(9)	-5(9)
F(2)	43(4)	91(10)	132(16)	80(11)	16(6)	9(5)
F(2A)	120(20)	47(6)	99(15)	7(7)	67(15)	-23(8)
F(3)	129(14)	89(7)	70(8)	-13(5)	80(9)	-25(7)
F(3A)	88(15)	153(24)	30(6)	18(9)	3(7)	-51(16)
F(4)	60(3)	127(4)	181(5)	-104(4)	-17(3)	-14(3)
F(5)	121(4)	39(2)	98(3)	-15(2)	-47(3)	12(2)
F(6)	353(10)	79(3)	30(2)	-18(2)	2(4)	-81(5)
O(1)	38(2)	39(2)	25(2)	0(1)	4(1)	-6(2)
O(2)	46(2)	33(2)	24(2)	-3(1)	1(1)	-7(2)
C(1)	56(3)	47(3)	29(2)	-8(2)	-1(2)	-18(3)
C(2)	84(5)	29(3)	36(3)	-7(2)	17(3)	-4(3)
C(3)	104(6)	54(4)	64(4)	-5(3)	34(4)	25(4)
C(4)	41(3)	82(5)	60(4)	8(3)	20(3)	19(3)
C(5)	36(3)	55(3)	37(3)	7(2)	6(2)	-9(2)
C(6)	53(3)	32(2)	28(2)	5(2)	7(2)	5(2)
C(7)	75(4)	57(4)	30(3)	10(2)	-11(3)	13(3)
C(8)	80(5)	80(5)	29(3)	1(3)	-18(3)	-9(4)
C(9)	34(3)	62(4)	33(3)	6(2)	7(2)	-3(2)
C(10)	25(2)	39(3)	25(2)	9(2)	-2(2)	3(2)
C(11)	43(3)	41(3)	19(2)	1(2)	3(2)	6(2)
C(12)	39(3)	35(2)	25(2)	-2(2)	-2(2)	6(2)
C(13)	69(4)	35(3)	33(3)	-6(2)	-8(2)	-5(3)
Ir'	28(1)	29(1)	26(1)	2(1)	-1(1)	3(1)
F(1')	123(4)	163(5)	39(2)	-2(2)	9(2)	88(4)
F(2')	91(3)	60(3)	99(3)	-38(2)	33(3)	-15(2)
F(3')	41(2)	104(3)	69(3)	-32(2)	21(2)	-10(2)
F(4')	102(15)	112(21)	58(9)	-32(10)	-47(9)	45(14)
F(4'A)	197(26)	115(14)	120(17)	24(14)	-112(18)	-72(18)
F(5')	43(6)	141(21)	59(7)	32(10)	-17(4)	18(8)
F(5'A)	187(24)	145(21)	59(7)	-8(9)	-39(11)	132(20)
F(6')	172(28)	95(17)	117(21)	83(16)	-91(20)	-61(18)
F(6'A)	95(8)	176(21)	43(5)	34(8)	-8(5)	43(11)
O(1')	34(2)	43(2)	32(2)	-3(1)	0(1)	7(2)
O(2')	41(2)	40(2)	30(2)	0(1)	-3(1)	10(2)
C(1')	53(3)	58(4)	28(2)	11(2)	-2(2)	20(3)
C(2')	44(3)	53(3)	35(3)	-15(2)	-15(2)	16(3)
C(3')	34(3)	77(5)	88(5)	-16(4)	-15(3)	-1(3)
C(4')	37(3)	106(6)	57(4)	-1(4)	15(3)	-9(3)
C(5')	42(3)	57(3)	33(3)	1(2)	6(2)	9(3)
C(6')	46(3)	36(3)	41(3)	-11(2)	-10(2)	14(2)
C(7')	82(5)	39(3)	77(5)	-2(3)	-20(4)	18(3)
C(8')	84(5)	42(3)	66(4)	17(3)	-13(4)	13(3)
C(9')	38(3)	59(3)	41(3)	-5(3)	5(2)	9(3)
C(10')	34(2)	30(2)	35(2)	-1(2)	5(2)	1(2)
C(11')	33(2)	36(3)	44(3)	0(2)	-6(2)	10(2)

C(12')	41(3)	34(3)	36(2)	4(2)	-9(2)	8(2)
C(13')	65(4)	66(4)	41(3)	0(3)	-19(3)	23(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(1A)	2147(4)	5174(4)	3532(2)	53
H(2A)	1080(4)	5822(3)	3281(3)	59
H(3A)	493(5)	5241(4)	4452(4)	89
H(3B)	45(5)	5821(4)	3950(4)	89
H(4A)	-614(4)	4821(5)	3544(3)	74
H(4B)	-461(4)	4439(5)	4257(3)	74
H(5A)	-201(3)	3508(4)	3294(3)	51
H(6A)	833(3)	2879(3)	3686(2)	45
H(7A)	818(4)	3943(4)	4726(3)	65
H(7B)	1439(4)	3239(4)	4617(3)	65
H(8A)	2310(5)	4108(5)	4272(3)	75
H(8B)	1823(5)	4746(5)	4696(3)	75
H(11A)	1639(3)	3791(3)	929(2)	41
H(1'A)	1170(4)	4481(4)	7563(2)	56
H(2'A)	534(3)	3346(4)	7767(3)	53
H(3'A)	-637(4)	4018(5)	8262(4)	80
H(3'B)	-397(4)	3137(5)	8539(4)	80
H(4'A)	-491(4)	3725(5)	9495(3)	79
H(4'B)	-408(4)	4626(5)	9192(3)	79
H(5'A)	706(3)	3861(4)	9896(3)	53
H(6'A)	1446(3)	4929(3)	9692(3)	49
H(7'A)	470(5)	5839(4)	9139(4)	79
H(7'B)	1325(5)	5900(4)	8880(4)	79
H(8'A)	799(5)	5739(4)	7923(3)	77
H(8'B)	58(5)	5317(4)	8224(3)	77
H(11B)	3501(3)	2391(3)	8770(2)	45



Thermogravimetric analysis (TGA, weight %) and differential scanning calorimetry (DSC, heat flow, mcal/sec) traces for the thermal analysis of (hfac)Ir(1,5-COD).

SEM image of an iridium film grown from (hfac)Ir(I)(1,5-COD) on a SiO_2 substrate at 350 °C.