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Bis[2-(3-methyl-2-pyridyl)phenyl-κ^2C^1,N](1,1,1-trifluoro-3-thenoylpropan-2-onato-κ^2O,O')iridium(III) ethyl acetate solvate

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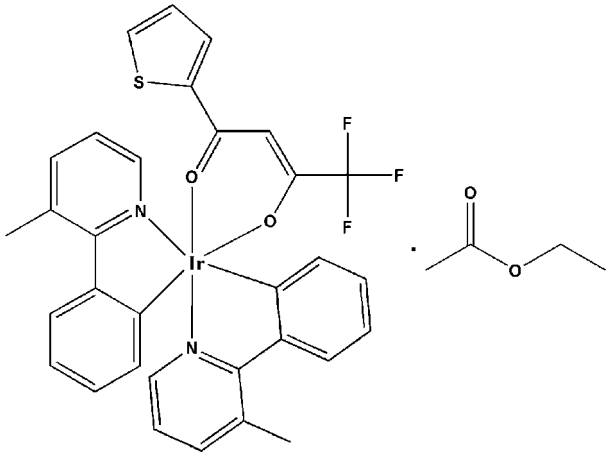
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.007 Å; R factor = 0.031; wR factor = 0.079; data-to-parameter ratio = 14.4.

The title compound, $[Ir(C_8H_4F_3O_2S)(C_{12}H_{10}N)_2]\cdot C_4H_8O_2$, contains two cyclometallated 3-methyl-2-phenylpyridine ligands and one thenoyltrifluoroacetonate ligand. The central Ir^{III} atom has a distorted octahedral coordination geometry, with the C atoms being *cis* and the N atoms *trans*.

Related literature

For related literature, see: DeRosa *et al.* (2004); Huo *et al.* (2006); Lamansky *et al.* (2001*a*,*b*); Lo *et al.* (2003); Xu *et al.* (2005).



Experimental

Crystal data

$[Ir(C_8H_4F_3O_2S)(C_{12}H_{10}N)_2]\cdot C_4H_8O_2$
M_r = 837.90
Triclinic, $P\overline{1}$
a = 11.4070 (8) Å
b = 12.889 (1) Å
c = 12.899 (2) Å
α = 68.874 (1)°
β = 65.149 (2)°
γ = 78.145 (1)°
V = 1601.9 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 4.29 mm^{-1}
T = 293 (2) K
0.49 × 0.32 × 0.19 mm

Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.211, T_{max} = 0.445
8980 measured reflections
6129 independent reflections
5681 reflections with $I > 2\sigma(I)$
R_{int} = 0.017

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.079
S = 1.05
6129 reflections
426 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 2.03 e Å^{-3}
$\Delta\rho_{min}$ = −0.98 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ir1—C26	1.982 (4)	Ir1—N1	2.041 (4)
Ir1—C20	1.986 (4)	Ir1—O1	2.170 (3)
Ir1—N2	2.036 (4)	Ir1—O2	2.171 (3)
C26—Ir1—C20	91.53 (16)	N2—Ir1—O1	95.88 (13)
C26—Ir1—N2	95.07 (16)	N1—Ir1—O1	87.11 (13)
C20—Ir1—N2	80.34 (16)	C26—Ir1—O2	174.81 (14)
C26—Ir1—N1	80.47 (16)	C20—Ir1—O2	92.52 (14)
C20—Ir1—N1	96.68 (17)	N2—Ir1—O2	88.82 (13)
N2—Ir1—N1	174.61 (13)	N1—Ir1—O2	95.81 (13)
C26—Ir1—O1	89.07 (14)	O1—Ir1—O2	87.11 (11)
C20—Ir1—O1	176.21 (15)		

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL-Plus* (Sheldrick, 1990); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HY2069).

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supplementary materials

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Bis[2-(3-methyl-2-pyridyl)phenyl-κ^2C^1,N](1,1,1-trifluoro-3-thenoylpropan-2-onato-κ^2O,O')iridium(III) ethyl acetate solvate

L.-P. Han, B. Li, J. Liu and J. Ying

Comment

In recent years, cyclometalated iridium complexes have been extensively investigated due to their promise as highly efficient phosphorescent emitters in organic light-emitting devices (OLEDs) (Lamansky *et al.*, 2001*b*; Huo *et al.*, 2006) and the other applications such as oxygen sensors (DeRosa *et al.*, 2004) and biological labeling reagents (Lo *et al.*, 2003). In general, heteroleptic cyclometalated iridium complexes have monoanionic derivatives of bidentate *o*-pyridylarene or *o*-pyridylheterocycle and ancillary ligands. In this paper, we utilize 3-methyl-2-phenylpyridine (mpp) as the cyclometalating ligand and thenoyltrifluoroacetone (tta) as the ancillary ligand to synthesize the title compound, (I). Compound (I) emits bright-yellow light under excitation of UV light, implying that it may find application in OLEDs as a highly efficient phosphorescent emitter.

Compound (I) shows a distorted octahedral coordination geometry around the Ir atom, formed by two mpp ligands and one tta ligand. The asymmetric unit contains one ethyl acetate solvent molecule (Fig. 1). The mpp ligands adopt a mutual eclipsed configuration with the N1 and N2 atoms residing at *trans* positions. The Ir—N distances are 2.041 (4)Å and 2.036 (4)Å (Table 1). The cyclometalated carbon atoms C20 and C26 are at *cis* positions with Ir—C distances of 1.986 (4)Å and 1.982 (4) Å. The Ir—C average bond distance (1.984 Å) is shorter than the Ir—N average bond distance (2.039 Å). This is similar to previously reported examples, including [$(ppy)_2$Ir(acac)], [$(tpy)_2$Ir(acac)] (Lamansky *et al.*, 2001*a*) and [$(dppy)_2$Ir(acac)] (Xu *et al.*, 2005). The tta ligand displays an O,*O*'-chelating coordination mode, and the distances of Ir—O are 2.170 (3)Å and 2.171 (3) Å. All other features appear to be normal.

Experimental

Compound (I) was obtained in two steps using standard method (Lamansky *et al.*, 2001*a*). $IrCl_3\cdot 3H_2O$ (0.178 g, 0.51 mmol), mpp (0.20 g, 1.26 mmol), 2-ethoxyethanol (9 ml) and water (3 ml) were heated to 393 K for 24 h under a nitrogen atmosphere. After cooling to room temperature, the precipitate was collected by filtration, washed with water and methanol, then vacuum dried. A mixture of the above-obtained chloride-bridged dimer (0.113 g, 0.10 mmol), tta (0.067 g, 0.25 mmol) and Na_2CO_3 (0.106 g, 1.0 mmol) in 2-ethoxyethanol (10 ml) was refluxed for 16 h under a nitrogen atmosphere. An excess of water was added after the solution was cooled to room temperature. Then the precipitate was collected by filtration and washed with methanol. The crude product was purified by column chromatography on silica gel with ethyl acetate/petroleum ether (1:10, *v*/*v*) as the eluent. Crystals suitable for X-ray diffraction were obtained by slow evaporation of the solvent.

Refinement

All H atoms were positioned geometrically and refined as riding atoms, with C—H = 0.93Å (CH), 0.97 Å (CH_2) and U_{iso}(H) = 1.2U_{eq}(C), and with C—H = 0.96 Å (CH_3) and U_{iso}(H) = 1.5U_{eq}(C). The highest residual electron density was found 0.88 Å from atom Ir1 and the deepest hole 0.55 Å from atom S1.

Figures

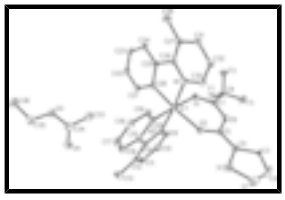

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

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Crystal data

$[Ir(C_8H_4F_3O_2S)(C_{12}H_{10}N)_2]\cdot C_4H_8O_2$	$Z = 2$
$M_r = 837.90$	$F_{000} = 828$
Triclinic, $P\overline{1}$	$D_x = 1.737$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71069$ Å
$a = 11.4070$ (8) Å	Cell parameters from 8940 reflections
$b = 12.889$ (1) Å	$\theta = 1.7$–26.0º
$c = 12.899$ (2) Å	$\mu = 4.29$ mm^{-1}
$\alpha = 68.874$ (1)º	$T = 293$ (2) K
$\beta = 65.149$ (2)º	Block, orange
$\gamma = 78.145$ (1)º	0.49 × 0.32 × 0.19 mm
$V = 1601.9$ (3) Å^3	

Data collection

Bruker APEX CCD area-detector diffractometer	6129 independent reflections
Radiation source: fine-focus sealed tube	5681 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.017$
$T = 293$(2) K	$\theta_{max} = 26.0$º
φ and ω scans	$\theta_{min} = 1.7$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -14\rightarrow13$
$T_{min} = 0.211$, $T_{max} = 0.445$	$k = -13\rightarrow15$
8980 measured reflections	$l = -15\rightarrow15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.031$	H-atom parameters constrained
$wR(F^2) = 0.079$	$w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 1.8469P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.05$	$(\Delta/\sigma)_{max} < 0.001$
6129 reflections	$\Delta\rho_{max} = 2.03$ e Å^{-3}
426 parameters	$\Delta\rho_{min} = -0.98$ e Å^{-3}
2 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ir1	0.179556 (14)	0.182767 (14)	0.202107 (14)	0.02173 (7)
C1	−0.4506 (5)	0.1622 (6)	0.4606 (5)	0.0518 (15)
H1	−0.5209	0.1660	0.5304	0.062*
C2	−0.4607 (5)	0.1454 (6)	0.3677 (6)	0.0580 (17)
H2	−0.5402	0.1363	0.3692	0.070*
C3	−0.3425 (3)	0.1421 (4)	0.2661 (3)	0.0172 (8)
H3	−0.3325	0.1311	0.1953	0.021*
C4	−0.2386 (4)	0.1603 (4)	0.2993 (4)	0.0278 (10)
C5	−0.0994 (4)	0.1644 (4)	0.2290 (4)	0.0252 (9)
C6	−0.0528 (4)	0.1541 (4)	0.1117 (4)	0.0292 (10)
H6	−0.1142	0.1440	0.0869	0.035*
C7	0.0726 (4)	0.1576 (4)	0.0320 (4)	0.0245 (9)
C8	0.1001 (5)	0.1527 (4)	−0.0932 (4)	0.0329 (11)
C9	0.1523 (4)	0.4130 (4)	0.0468 (4)	0.0309 (10)
H9	0.1550	0.3765	−0.0046	0.037*
C10	0.1436 (5)	0.5277 (4)	0.0097 (4)	0.0339 (11)
H10	0.1412	0.5686	−0.0654	0.041*
C11	0.1385 (4)	0.5796 (4)	0.0885 (4)	0.0328 (11)
H11	0.1319	0.6571	0.0659	0.039*
C12	0.1431 (4)	0.5198 (4)	0.2002 (4)	0.0281 (10)
C13	0.1340 (6)	0.5842 (4)	0.2803 (5)	0.0425 (13)
H13A	0.0700	0.5541	0.3588	0.064*
H13B	0.1097	0.6611	0.2472	0.064*
H13C	0.2164	0.5787	0.2860	0.064*
C14	0.1546 (4)	0.4016 (4)	0.2325 (4)	0.0239 (9)
C15	0.1677 (4)	0.3197 (4)	0.3417 (4)	0.0259 (9)
C16	0.1711 (5)	0.3449 (4)	0.4377 (4)	0.0346 (11)
H16	0.1633	0.4190	0.4352	0.041*
C17	0.1856 (5)	0.2623 (5)	0.5349 (4)	0.0378 (12)
H17	0.1881	0.2806	0.5974	0.045*
C18	0.1965 (5)	0.1513 (4)	0.5405 (4)	0.0336 (11)
H18	0.2056	0.0951	0.6069	0.040*
C19	0.1939 (4)	0.1246 (4)	0.4467 (4)	0.0279 (10)
H19	0.2012	0.0501	0.4512	0.034*
C20	0.1806 (4)	0.2066 (4)	0.3455 (4)	0.0231 (9)
C21	0.4492 (4)	0.2668 (4)	0.0572 (4)	0.0288 (10)
H21	0.4120	0.3388	0.0530	0.035*

C22	0.5807 (4)	0.2517 (4)	−0.0065 (4)	0.0334 (11)
H22	0.6300	0.3134	−0.0523	0.040*
C23	0.6388 (4)	0.1474 (4)	−0.0031 (4)	0.0309 (10)
H23	0.7265	0.1385	−0.0483	0.037*
C24	0.5660 (4)	0.0538 (4)	0.0688 (4)	0.0274 (10)
H24	0.6058	−0.0173	0.0722	0.033*
C25	0.4329 (4)	0.0672 (4)	0.1357 (4)	0.0226 (9)
C26	0.3713 (4)	0.1768 (4)	0.1274 (4)	0.0239 (9)
C27	0.3776 (4)	−0.1393 (4)	0.2521 (4)	0.0271 (9)
C28	0.5152 (5)	−0.1895 (4)	0.2198 (5)	0.0406 (12)
H28A	0.5679	−0.1444	0.2260	0.061*
H28B	0.5483	−0.1924	0.1390	0.061*
H28C	0.5168	−0.2635	0.2740	0.061*
C29	0.3453 (4)	−0.0242 (4)	0.2139 (4)	0.0229 (9)
C30	0.1236 (4)	−0.0567 (4)	0.3240 (4)	0.0321 (10)
H30	0.0379	−0.0284	0.3490	0.039*
C31	0.2778 (5)	−0.2102 (4)	0.3241 (4)	0.0301 (10)
H31	0.2973	−0.2867	0.3479	0.036*
C32	0.1501 (5)	−0.1699 (4)	0.3613 (5)	0.0333 (11)
H32	0.0838	−0.2180	0.4102	0.040*
C33	0.5052 (6)	0.4418 (5)	0.1911 (5)	0.0485 (14)
H33A	0.5880	0.4156	0.1427	0.073*
H33B	0.4713	0.5040	0.1409	0.073*
H33C	0.4467	0.3830	0.2306	0.073*
C34	0.5199 (5)	0.4769 (5)	0.2825 (5)	0.0419 (13)
C35	0.6654 (6)	0.4854 (6)	0.3667 (6)	0.0528 (15)
H35A	0.6182	0.4364	0.4456	0.063*
H35B	0.6363	0.5618	0.3658	0.063*
C36	0.8079 (6)	0.4676 (6)	0.3401 (7)	0.0622 (18)
H36A	0.8254	0.4827	0.3997	0.093*
H36B	0.8538	0.5168	0.2622	0.093*
H36C	0.8358	0.3917	0.3414	0.093*
N1	0.2178 (3)	0.0142 (3)	0.2525 (3)	0.0241 (8)
N2	0.1569 (3)	0.3522 (3)	0.1535 (3)	0.0227 (7)
O1	0.1758 (3)	0.1685 (3)	0.0410 (3)	0.0278 (7)
O2	−0.0296 (3)	0.1773 (3)	0.2775 (3)	0.0271 (7)
O3	0.6419 (3)	0.4617 (3)	0.2760 (3)	0.0444 (9)
O4	0.4318 (4)	0.5138 (4)	0.3568 (4)	0.0575 (12)
F1	0.1508 (4)	0.2460 (3)	−0.1773 (3)	0.0559 (9)
F2	0.1846 (3)	0.0694 (3)	−0.1195 (3)	0.0480 (8)
F3	−0.0050 (3)	0.1408 (3)	−0.1090 (3)	0.0494 (8)
S1	−0.29934 (14)	0.17557 (14)	0.43745 (14)	0.0497 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ir1	0.01775 (10)	0.02274 (10)	0.02497 (10)	−0.00244 (6)	−0.00687 (7)	−0.00852 (7)
C1	0.031 (3)	0.065 (4)	0.042 (3)	−0.003 (3)	−0.001 (2)	−0.014 (3)

C2	0.029 (3)	0.081 (5)	0.061 (4)	−0.012 (3)	−0.018 (3)	−0.014 (4)
C3	0.0035 (15)	0.033 (2)	0.0139 (18)	−0.0038 (15)	0.0005 (14)	−0.0089 (17)
C4	0.025 (2)	0.027 (2)	0.029 (2)	−0.0033 (18)	−0.0080 (19)	−0.0073 (19)
C5	0.024 (2)	0.018 (2)	0.030 (2)	0.0006 (17)	−0.0099 (19)	−0.0055 (18)
C6	0.029 (2)	0.027 (2)	0.033 (2)	−0.0018 (19)	−0.014 (2)	−0.009 (2)
C7	0.027 (2)	0.019 (2)	0.030 (2)	0.0022 (17)	−0.0133 (19)	−0.0090 (18)
C8	0.029 (2)	0.039 (3)	0.037 (3)	0.000 (2)	−0.015 (2)	−0.016 (2)
C9	0.032 (2)	0.033 (3)	0.030 (2)	−0.001 (2)	−0.014 (2)	−0.009 (2)
C10	0.032 (2)	0.035 (3)	0.033 (3)	−0.001 (2)	−0.015 (2)	−0.006 (2)
C11	0.025 (2)	0.025 (2)	0.041 (3)	0.0006 (19)	−0.012 (2)	−0.004 (2)
C12	0.019 (2)	0.026 (2)	0.038 (3)	−0.0028 (18)	−0.0075 (19)	−0.013 (2)
C13	0.054 (3)	0.026 (3)	0.048 (3)	−0.001 (2)	−0.018 (3)	−0.015 (2)
C14	0.0167 (19)	0.026 (2)	0.029 (2)	0.0000 (17)	−0.0088 (17)	−0.0094 (19)
C15	0.018 (2)	0.030 (2)	0.028 (2)	−0.0036 (18)	−0.0049 (17)	−0.0106 (19)
C16	0.041 (3)	0.035 (3)	0.029 (2)	−0.007 (2)	−0.011 (2)	−0.011 (2)
C17	0.041 (3)	0.051 (3)	0.027 (2)	−0.010 (2)	−0.012 (2)	−0.015 (2)
C18	0.031 (2)	0.040 (3)	0.027 (2)	−0.005 (2)	−0.012 (2)	−0.004 (2)
C19	0.024 (2)	0.027 (2)	0.031 (2)	−0.0030 (18)	−0.0099 (19)	−0.006 (2)
C20	0.0122 (18)	0.030 (2)	0.024 (2)	−0.0023 (17)	−0.0044 (16)	−0.0076 (18)
C21	0.026 (2)	0.029 (2)	0.034 (2)	−0.0040 (19)	−0.0127 (19)	−0.010 (2)
C22	0.028 (2)	0.043 (3)	0.028 (2)	−0.014 (2)	−0.0089 (19)	−0.005 (2)
C23	0.021 (2)	0.047 (3)	0.028 (2)	−0.001 (2)	−0.0089 (18)	−0.016 (2)
C24	0.024 (2)	0.034 (3)	0.026 (2)	0.0005 (19)	−0.0122 (18)	−0.009 (2)
C25	0.020 (2)	0.030 (2)	0.023 (2)	−0.0020 (18)	−0.0094 (17)	−0.0124 (19)
C26	0.021 (2)	0.032 (2)	0.025 (2)	−0.0046 (18)	−0.0116 (17)	−0.0094 (19)
C27	0.032 (2)	0.026 (2)	0.026 (2)	0.0008 (19)	−0.0125 (19)	−0.0099 (19)
C28	0.035 (3)	0.032 (3)	0.050 (3)	0.005 (2)	−0.017 (2)	−0.010 (2)
C29	0.022 (2)	0.030 (2)	0.024 (2)	0.0008 (18)	−0.0104 (17)	−0.0152 (19)
C30	0.024 (2)	0.033 (3)	0.039 (3)	−0.007 (2)	−0.009 (2)	−0.011 (2)
C31	0.034 (2)	0.023 (2)	0.033 (2)	−0.003 (2)	−0.012 (2)	−0.009 (2)
C32	0.032 (2)	0.027 (2)	0.040 (3)	−0.010 (2)	−0.010 (2)	−0.009 (2)
C33	0.044 (3)	0.054 (4)	0.046 (3)	−0.008 (3)	−0.018 (3)	−0.011 (3)
C34	0.041 (3)	0.032 (3)	0.046 (3)	−0.007 (2)	−0.016 (3)	−0.003 (2)
C35	0.044 (3)	0.063 (4)	0.059 (4)	0.001 (3)	−0.021 (3)	−0.029 (3)
C36	0.044 (3)	0.066 (4)	0.083 (5)	−0.006 (3)	−0.027 (3)	−0.026 (4)
N1	0.0194 (17)	0.0236 (19)	0.030 (2)	−0.0023 (15)	−0.0071 (15)	−0.0104 (16)
N2	0.0173 (17)	0.0216 (18)	0.0271 (19)	−0.0003 (14)	−0.0068 (14)	−0.0077 (15)
O1	0.0233 (15)	0.0345 (18)	0.0269 (16)	−0.0026 (13)	−0.0074 (13)	−0.0130 (14)
O2	0.0217 (15)	0.0330 (18)	0.0286 (16)	−0.0008 (13)	−0.0104 (13)	−0.0113 (14)
O3	0.0309 (19)	0.055 (2)	0.047 (2)	0.0013 (17)	−0.0129 (17)	−0.0194 (19)
O4	0.038 (2)	0.072 (3)	0.072 (3)	0.001 (2)	−0.012 (2)	−0.045 (3)
F1	0.077 (2)	0.058 (2)	0.0277 (16)	−0.0214 (19)	−0.0157 (16)	−0.0037 (15)
F2	0.0417 (17)	0.062 (2)	0.056 (2)	0.0156 (16)	−0.0233 (15)	−0.0395 (18)
F3	0.0341 (16)	0.083 (3)	0.0493 (18)	0.0040 (16)	−0.0215 (14)	−0.0375 (18)
S1	0.0400 (7)	0.0617 (10)	0.0450 (8)	−0.0041 (7)	−0.0121 (6)	−0.0181 (7)

Geometric parameters (Å, °)

Ir1—C26	1.982 (4)	C17—H17	0.9300

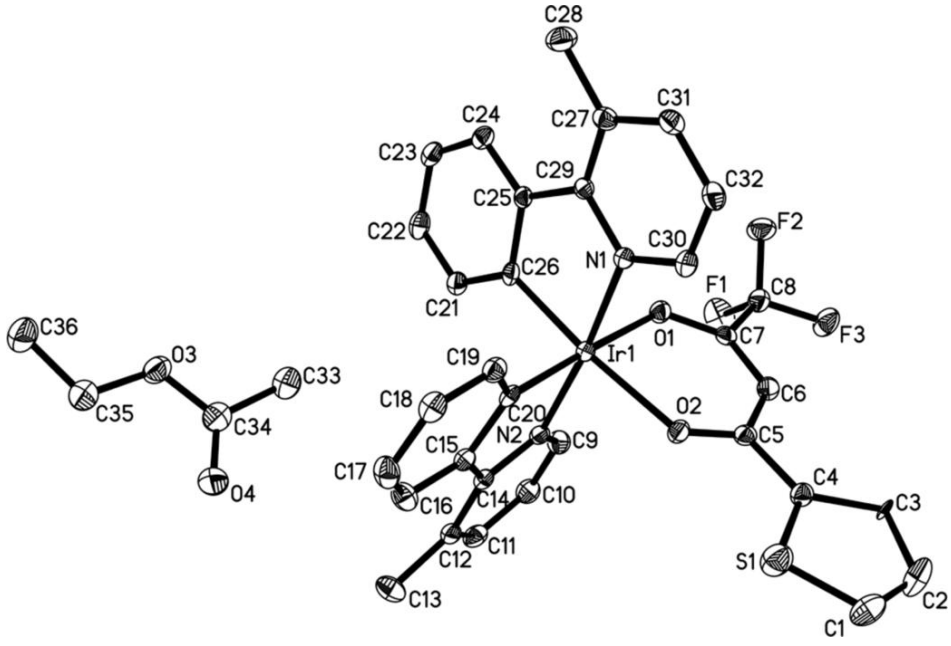
Ir1—C20	1.986 (4)	C18—C19	1.385 (7)
Ir1—N2	2.036 (4)	C18—H18	0.9300
Ir1—N1	2.041 (4)	C19—C20	1.397 (6)
Ir1—O1	2.170 (3)	C19—H19	0.9300
Ir1—O2	2.171 (3)	C21—C22	1.386 (6)
C1—C2	1.346 (9)	C21—C26	1.395 (6)
C1—S1	1.657 (6)	C21—H21	0.9300
C1—H1	0.9300	C22—C23	1.365 (7)
C2—C3	1.439 (7)	C22—H22	0.9300
C2—H2	0.9300	C23—C24	1.400 (7)
C3—C4	1.501 (6)	C23—H23	0.9300
C3—H3	0.9300	C24—C25	1.407 (6)
C4—C5	1.462 (6)	C24—H24	0.9300
C4—S1	1.690 (5)	C25—C26	1.431 (6)
C5—O2	1.266 (5)	C25—C29	1.477 (6)
C5—C6	1.424 (6)	C27—C31	1.386 (7)
C6—C7	1.365 (6)	C27—C29	1.407 (6)
C6—H6	0.9300	C27—C28	1.511 (7)
C7—O1	1.271 (5)	C28—H28A	0.9600
C7—C8	1.532 (6)	C28—H28B	0.9600
C8—F2	1.327 (6)	C28—H28C	0.9600
C8—F1	1.332 (6)	C29—N1	1.372 (5)
C8—F3	1.343 (5)	C30—N1	1.343 (6)
C9—N2	1.333 (6)	C30—C32	1.373 (7)
C9—C10	1.375 (7)	C30—H30	0.9300
C9—H9	0.9300	C31—C32	1.379 (7)
C10—C11	1.383 (7)	C31—H31	0.9300
C10—H10	0.9300	C32—H32	0.9300
C11—C12	1.385 (7)	C33—C34	1.486 (8)
C11—H11	0.9300	C33—H33A	0.9600
C12—C14	1.421 (6)	C33—H33B	0.9600
C12—C13	1.503 (7)	C33—H33C	0.9600
C13—H13A	0.9600	C34—O4	1.215 (7)
C13—H13B	0.9600	C34—O3	1.336 (6)
C13—H13C	0.9600	C35—O3	1.445 (7)
C14—N2	1.373 (5)	C35—C36	1.499 (8)
C14—C15	1.470 (6)	C35—H35A	0.9700
C15—C16	1.405 (6)	C35—H35B	0.9700
C15—C20	1.420 (6)	C36—H36A	0.9600
C16—C17	1.368 (7)	C36—H36B	0.9600
C16—H16	0.9300	C36—H36C	0.9600
C17—C18	1.388 (7)		
C26—Ir1—C20	91.53 (16)	C18—C19—H19	119.1
C26—Ir1—N2	95.07 (16)	C20—C19—H19	119.1
C20—Ir1—N2	80.34 (16)	C19—C20—C15	117.9 (4)
C26—Ir1—N1	80.47 (16)	C19—C20—Ir1	126.9 (3)
C20—Ir1—N1	96.68 (17)	C15—C20—Ir1	115.3 (3)
N2—Ir1—N1	174.61 (13)	C22—C21—C26	121.7 (5)
C26—Ir1—O1	89.07 (14)	C22—C21—H21	119.2

C20—Ir1—O1	176.21 (15)	C26—C21—H21	119.2
N2—Ir1—O1	95.88 (13)	C23—C22—C21	120.9 (5)
N1—Ir1—O1	87.11 (13)	C23—C22—H22	119.5
C26—Ir1—O2	174.81 (14)	C21—C22—H22	119.5
C20—Ir1—O2	92.52 (14)	C22—C23—C24	119.8 (4)
N2—Ir1—O2	88.82 (13)	C22—C23—H23	120.1
N1—Ir1—O2	95.81 (13)	C24—C23—H23	120.1
O1—Ir1—O2	87.11 (11)	C23—C24—C25	120.2 (4)
C2—C1—S1	112.8 (4)	C23—C24—H24	119.9
C2—C1—H1	123.6	C25—C24—H24	119.9
S1—C1—H1	123.6	C24—C25—C26	119.8 (4)
C1—C2—C3	116.7 (5)	C24—C25—C29	125.5 (4)
C1—C2—H2	121.6	C26—C25—C29	114.7 (4)
C3—C2—H2	121.6	C21—C26—C25	117.5 (4)
C2—C3—C4	104.9 (4)	C21—C26—Ir1	127.0 (4)
C2—C3—H3	127.6	C25—C26—Ir1	115.0 (3)
C4—C3—H3	127.6	C31—C27—C29	118.2 (4)
C5—C4—C3	128.3 (4)	C31—C27—C28	118.3 (4)
C5—C4—S1	119.7 (3)	C29—C27—C28	123.5 (4)
C3—C4—S1	111.9 (3)	C27—C28—H28A	109.5
O2—C5—C6	125.1 (4)	C27—C28—H28B	109.5
O2—C5—C4	117.0 (4)	H28A—C28—H28B	109.5
C6—C5—C4	117.8 (4)	C27—C28—H28C	109.5
C7—C6—C5	126.7 (4)	H28A—C28—H28C	109.5
C7—C6—H6	116.7	H28B—C28—H28C	109.5
C5—C6—H6	116.7	N1—C29—C27	119.3 (4)
O1—C7—C6	130.8 (4)	N1—C29—C25	112.2 (4)
O1—C7—C8	111.1 (4)	C27—C29—C25	128.5 (4)
C6—C7—C8	118.0 (4)	N1—C30—C32	121.8 (4)
F2—C8—F1	106.6 (4)	N1—C30—H30	119.1
F2—C8—F3	106.3 (4)	C32—C30—H30	119.1
F1—C8—F3	106.3 (4)	C32—C31—C27	121.4 (5)
F2—C8—C7	112.2 (4)	C32—C31—H31	119.3
F1—C8—C7	110.6 (4)	C27—C31—H31	119.3
F3—C8—C7	114.3 (4)	C30—C32—C31	118.2 (4)
N2—C9—C10	122.7 (4)	C30—C32—H32	120.9
N2—C9—H9	118.6	C31—C32—H32	120.9
C10—C9—H9	118.6	C34—C33—H33A	109.5
C9—C10—C11	117.3 (4)	C34—C33—H33B	109.5
C9—C10—H10	121.4	H33A—C33—H33B	109.5
C11—C10—H10	121.4	C34—C33—H33C	109.5
C10—C11—C12	122.0 (5)	H33A—C33—H33C	109.5
C10—C11—H11	119.0	H33B—C33—H33C	109.5
C12—C11—H11	119.0	O4—C34—O3	122.9 (5)
C11—C12—C14	118.1 (4)	O4—C34—C33	124.7 (5)
C11—C12—C13	117.8 (4)	O3—C34—C33	112.4 (5)
C14—C12—C13	124.1 (4)	O3—C35—C36	108.3 (5)
C12—C13—H13A	109.5	O3—C35—H35A	110.0
C12—C13—H13B	109.5	C36—C35—H35A	110.0

H13A—C13—H13B	109.5	O3—C35—H35B	110.0
C12—C13—H13C	109.5	C36—C35—H35B	110.0
H13A—C13—H13C	109.5	H35A—C35—H35B	108.4
H13B—C13—H13C	109.5	C35—C36—H36A	109.5
N2—C14—C12	118.7 (4)	C35—C36—H36B	109.5
N2—C14—C15	112.5 (4)	H36A—C36—H36B	109.5
C12—C14—C15	128.9 (4)	C35—C36—H36C	109.5
C16—C15—C20	119.3 (4)	H36A—C36—H36C	109.5
C16—C15—C14	125.7 (4)	H36B—C36—H36C	109.5
C20—C15—C14	115.0 (4)	C30—N1—C29	120.9 (4)
C17—C16—C15	121.1 (5)	C30—N1—Ir1	122.0 (3)
C17—C16—H16	119.5	C29—N1—Ir1	117.0 (3)
C15—C16—H16	119.5	C9—N2—C14	121.2 (4)
C16—C17—C18	120.2 (5)	C9—N2—Ir1	121.8 (3)
C16—C17—H17	119.9	C14—N2—Ir1	116.9 (3)
C18—C17—H17	119.9	C7—O1—Ir1	123.1 (3)
C19—C18—C17	119.6 (5)	C5—O2—Ir1	127.0 (3)
C19—C18—H18	120.2	C34—O3—C35	116.9 (4)
C17—C18—H18	120.2	C1—S1—C4	93.7 (3)
C18—C19—C20	121.9 (5)		
S1—C1—C2—C3	−0.2 (8)	O1—Ir1—C26—C21	90.3 (4)
C1—C2—C3—C4	−0.2 (7)	C20—Ir1—C26—C25	102.1 (3)
C2—C3—C4—C5	179.7 (5)	N2—Ir1—C26—C25	−177.5 (3)
C2—C3—C4—S1	0.5 (5)	N1—Ir1—C26—C25	5.5 (3)
C3—C4—C5—O2	−177.8 (4)	O1—Ir1—C26—C25	−81.7 (3)
S1—C4—C5—O2	1.4 (6)	C31—C27—C29—N1	2.5 (6)
C3—C4—C5—C6	2.5 (7)	C28—C27—C29—N1	−176.8 (4)
S1—C4—C5—C6	−178.3 (3)	C31—C27—C29—C25	−178.7 (4)
O2—C5—C6—C7	−0.8 (8)	C28—C27—C29—C25	2.0 (7)
C4—C5—C6—C7	178.9 (4)	C24—C25—C29—N1	−170.4 (4)
C5—C6—C7—O1	1.2 (8)	C26—C25—C29—N1	7.3 (5)
C5—C6—C7—C8	−175.9 (4)	C24—C25—C29—C27	10.8 (7)
O1—C7—C8—F2	58.6 (5)	C26—C25—C29—C27	−171.5 (4)
C6—C7—C8—F2	−123.8 (5)	C29—C27—C31—C32	−2.1 (7)
O1—C7—C8—F1	−60.3 (5)	C28—C27—C31—C32	177.2 (4)
C6—C7—C8—F1	117.3 (5)	N1—C30—C32—C31	0.5 (7)
O1—C7—C8—F3	179.8 (4)	C27—C31—C32—C30	0.6 (7)
C6—C7—C8—F3	−2.6 (6)	C32—C30—N1—C29	−0.1 (7)
N2—C9—C10—C11	−0.5 (7)	C32—C30—N1—Ir1	−177.6 (4)
C9—C10—C11—C12	0.5 (7)	C27—C29—N1—C30	−1.4 (6)
C10—C11—C12—C14	0.7 (7)	C25—C29—N1—C30	179.6 (4)
C10—C11—C12—C13	−178.7 (4)	C27—C29—N1—Ir1	176.2 (3)
C11—C12—C14—N2	−1.9 (6)	C25—C29—N1—Ir1	−2.8 (4)
C13—C12—C14—N2	177.4 (4)	C26—Ir1—N1—C30	176.1 (4)
C11—C12—C14—C15	176.7 (4)	C20—Ir1—N1—C30	85.7 (4)
C13—C12—C14—C15	−4.0 (7)	O1—Ir1—N1—C30	−94.3 (4)
N2—C14—C15—C16	178.8 (4)	O2—Ir1—N1—C30	−7.5 (4)
C12—C14—C15—C16	0.1 (7)	C26—Ir1—N1—C29	−1.5 (3)
N2—C14—C15—C20	0.2 (5)	C20—Ir1—N1—C29	−91.9 (3)

C12—C14—C15—C20	−178.5 (4)	O1—Ir1—N1—C29	88.1 (3)
C20—C15—C16—C17	−0.5 (7)	O2—Ir1—N1—C29	174.9 (3)
C14—C15—C16—C17	−179.0 (4)	C10—C9—N2—C14	−0.7 (7)
C15—C16—C17—C18	−0.4 (8)	C10—C9—N2—Ir1	−176.6 (3)
C16—C17—C18—C19	0.6 (8)	C12—C14—N2—C9	1.9 (6)
C17—C18—C19—C20	0.1 (7)	C15—C14—N2—C9	−176.9 (4)
C18—C19—C20—C15	−0.9 (6)	C12—C14—N2—Ir1	178.0 (3)
C18—C19—C20—Ir1	178.3 (3)	C15—C14—N2—Ir1	−0.8 (4)
C16—C15—C20—C19	1.1 (6)	C26—Ir1—N2—C9	86.2 (4)
C14—C15—C20—C19	179.8 (4)	C20—Ir1—N2—C9	176.9 (4)
C16—C15—C20—Ir1	−178.2 (3)	O1—Ir1—N2—C9	−3.4 (3)
C14—C15—C20—Ir1	0.5 (5)	O2—Ir1—N2—C9	−90.4 (3)
C26—Ir1—C20—C19	−85.0 (4)	C26—Ir1—N2—C14	−89.9 (3)
N2—Ir1—C20—C19	−179.9 (4)	C20—Ir1—N2—C14	0.8 (3)
N1—Ir1—C20—C19	−4.4 (4)	O1—Ir1—N2—C14	−179.5 (3)
O2—Ir1—C20—C19	91.7 (4)	O2—Ir1—N2—C14	93.6 (3)
C26—Ir1—C20—C15	94.2 (3)	C6—C7—O1—Ir1	1.3 (7)
N2—Ir1—C20—C15	−0.7 (3)	C8—C7—O1—Ir1	178.5 (3)
N1—Ir1—C20—C15	174.8 (3)	C26—Ir1—O1—C7	173.9 (4)
O2—Ir1—C20—C15	−89.1 (3)	N2—Ir1—O1—C7	−91.1 (4)
C26—C21—C22—C23	0.2 (7)	N1—Ir1—O1—C7	93.4 (4)
C21—C22—C23—C24	−2.1 (7)	O2—Ir1—O1—C7	−2.6 (3)
C22—C23—C24—C25	1.0 (7)	C6—C5—O2—Ir1	−2.0 (6)
C23—C24—C25—C26	1.9 (6)	C4—C5—O2—Ir1	178.3 (3)
C23—C24—C25—C29	179.5 (4)	C20—Ir1—O2—C5	179.3 (4)
C22—C21—C26—C25	2.6 (6)	N2—Ir1—O2—C5	99.0 (4)
C22—C21—C26—Ir1	−169.2 (3)	N1—Ir1—O2—C5	−83.7 (4)
C24—C25—C26—C21	−3.6 (6)	O1—Ir1—O2—C5	3.1 (4)
C29—C25—C26—C21	178.5 (4)	O4—C34—O3—C35	3.4 (8)
C24—C25—C26—Ir1	169.1 (3)	C33—C34—O3—C35	−175.5 (5)
C29—C25—C26—Ir1	−8.7 (5)	C36—C35—O3—C34	−177.7 (5)
C20—Ir1—C26—C21	−86.0 (4)	C2—C1—S1—C4	0.5 (6)
N2—Ir1—C26—C21	−5.6 (4)	C5—C4—S1—C1	−179.8 (4)
N1—Ir1—C26—C21	177.5 (4)	C3—C4—S1—C1	−0.5 (4)

Fig. 1


C28
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