Acta Cryst E
CRYSTALLOGRAPHIC
COMMUNICATIONS

ISSN 2056-9890

Crystal structure of chlorido(dimethyl sulfoxide-κS)bis[4-(pyridin-2-yl)benzaldehyde-κ^3C^2,N]-iridium(III) acetonitrile monosolvate

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Received 20 June 2017
Accepted 25 July 2017

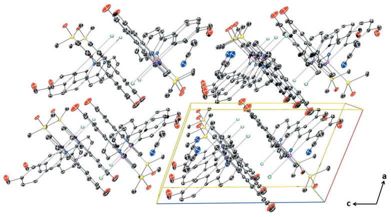
Edited by M. Weil, Vienna University of Technology, Austria

Keywords: crystal structure; iridium; phenylpyridine derivative.

CCDC reference: 1564599

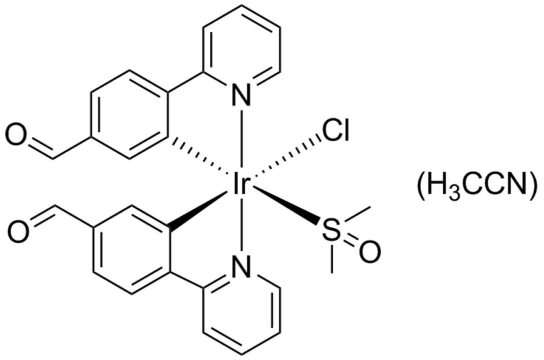
Supporting information: this article has supporting information at journals.iucr.org/e

The title compound, $[IrCl(C_{12}H_8NO)_2\{(CH_3)_2SO\}]\cdot H_3CCN$ or $[IrCl(fppy)_2(DMSO)]\cdot H_3CCN$ [where fppy is 4-(pyridin-2-yl)benzaldehyde and DMSO is dimethyl sulfoxide], is a mononuclear iridium(III) complex including two fppy ligands, a sulfur-coordinating DMSO ligand, and one terminal chloride ligand that define a distorted octahedral coordination sphere. The complex crystallizes from 1:1 DMSO–acetonitrile as an acetonitrile solvate. In the crystal, weak C—H⋯O and C—H⋯N hydrogen-bonding interactions between adjacent complexes and between the acetonitrile solvent and the complex consolidate the packing.



1. Chemical context

The development of iridium complexes with three *ortho* metallating ligands has drawn great interest due to their potential application in light-emitting devices (Henwood & Zysman-Coman, 2017). Many such complexes have been synthesized, often utilizing phenylpyridine-based dichlorido-bridged di-iridium complexes as starting materials. In an attempt to synthesize such a compound with 4-(pyridin-2-yl)benzaldehyde (fppy) as a ligand, *viz*. di-μ-chlorido-bis-{bis[4-(pyridin-2-yl)benzaldehyde-κ^2C^2,N']iridium(III) (Bettington *et al.*, 2004), spectroscopic results indicated a product with reduced symmetry compared to the expected C_i symmetry of the known complex. Single-crystal X-ray analysis was used to elucidate the structure of the title compound.



2. Structural commentary

The title compound (Fig. 1) crystallizes in the triclinic space group $P\overline{1}$ with one molecule per asymmetric unit. The Ir^{III} atom has a distorted octahedral coordination sphere defined

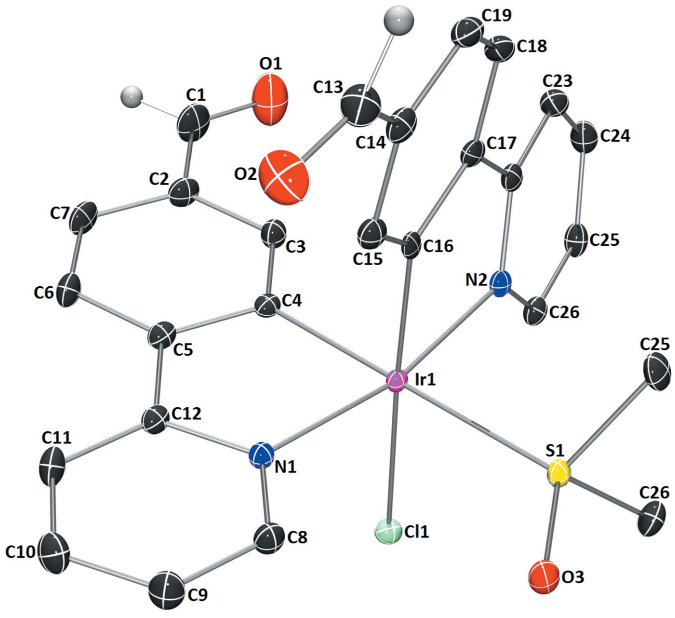


Figure 1
The molecular structure of chlorido(dimethyl sulfoxide-κS)bis[4-(pyridin-2-yl)benzaldehyde-κ^2C^2,N']iridium(III) acetonitrile monosolvate. Displacement ellipsoids are shown at the 50% probability level. Only aldehyde H atoms are shown and the acetonitrile solvent molecule has been omitted for clarity.

Table 1
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C19—H19$\cdots$O3^{i}	0.93	2.48	3.179 (3)	132
C25—H25$B\cdots$N3^{ii}	0.96	2.53	3.403 (3)	150
C26—H26$A\cdots$O3^{iii}	0.96	2.48	3.406 (2)	161
C28—H28$C\cdots$O1^{iv}	0.96	2.54	3.490 (3)	173

Symmetry codes: (i) $x-1, y, z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x+2, -y+2, -z+2$; (iv) $x+1, y, z$.

by the S atom of the dimethyl sulfoxide (DMSO) ligand, a chlorine ligand and C and N atoms of two fppy ligands. The S and Cl atoms occupy equatorial positions, *trans* to the fppy C atoms, and the fppy N atoms occupy the axial positions. The least-squares planes of each fppy ligand indicate a nearly coplanar arrangement of the pyridine and phenyl rings with small deviations of 2.42 (9)° (fppy ligand N1/C2–C12 with C4 *trans* to S1) and 14.71 (9)° (fppy ligand N2/C14–C24 with C16 *trans* to Cl1). The Ir—S bond length [2.3810 (5) Å] is longer than the average distance [2.27 (1) Å] that was reported for this coordination mode (Calligaris, 2004). The S—O distance [1.4903 (13) Å] is only slightly longer than the previously reported average [1.473 (4) Å]. This S—O distance shows negligible contraction from the average reported S—O bond length [1.492 (1) Å] in non-coordinating sulfoxide molecules (Calligaris, 2004).

3. Supramolecular features

The acetonitrile solvate molecules fill voids that are visible along the *b* axis view direction (Fig. 2). Alignment of the

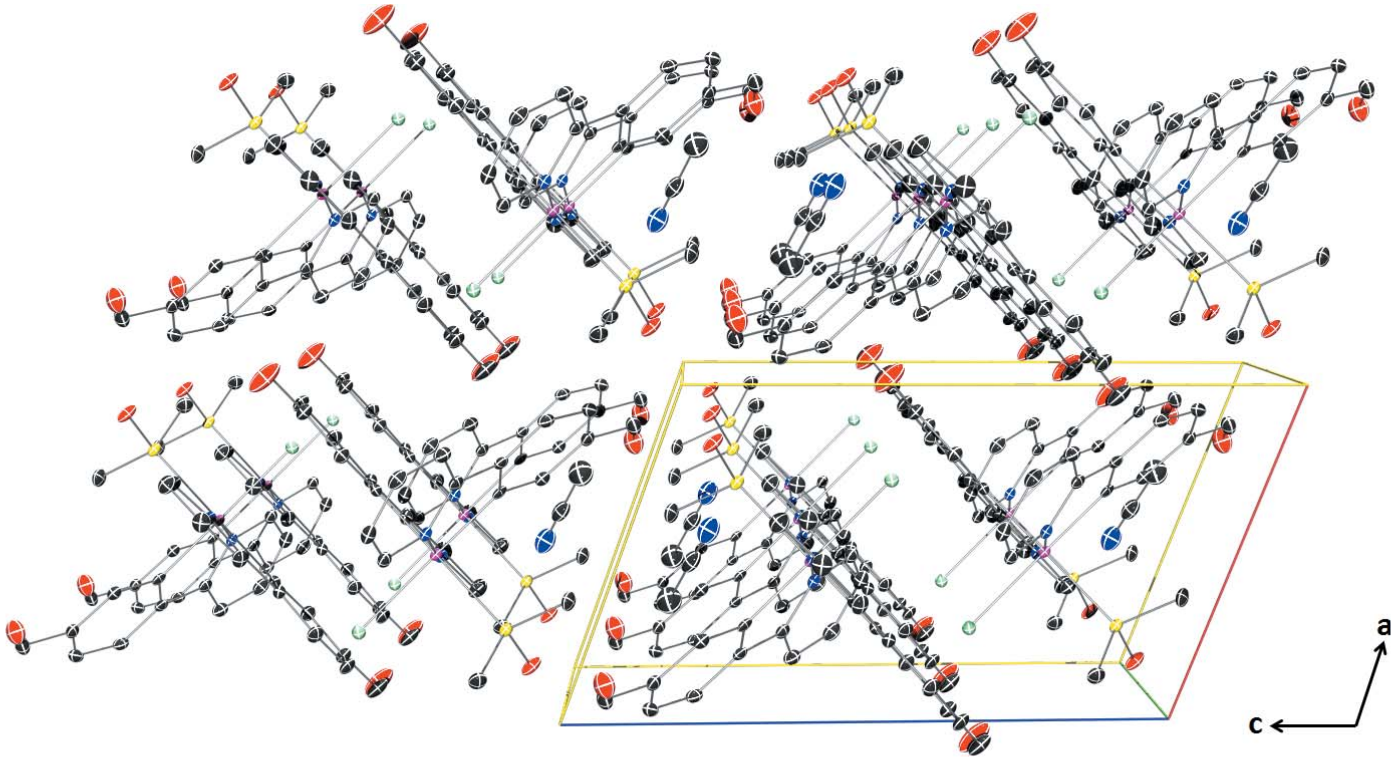


Figure 2
The crystal packing of the title complex, viewed along the *b* axis. Displacement ellipsoids are shown at the 50% probability level. H atoms have been omitted for clarity.

Table 2
Experimental details.

Crystal data	
Chemical formula	$[\mathrm{IrCl(C_{12}H_8NO)_2(C_2H_6OS)}]\cdot\mathrm{C_2H_3N}$
M_r	711.22
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	8.7837 (12), 12.0910 (16), 14.0097 (19)
α, β, γ (°)	97.5367 (15), 105.1501 (14), 109.3176 (14)
V (Å^3)	1316.1 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.29
Crystal size (mm)	0.32 × 0.24 × 0.17
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
$T_{\min}$, $T_{\max}$	0.26, 0.47
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	28976, 6983, 6828
$R_{\rm int}$	0.026
$(\sin \theta/\lambda)_{\max}$ (Å^{-1})	0.685
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.015, 0.037, 1.68
No. of reflections	6983
No. of parameters	345
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å^{-3})	1.47, −0.65

Computer programs: *APEX3* and *SAINT* (Bruker, 2017), *SHELXS* (Sheldrick, 2008), *SHELXL2016* (Sheldrick, 2015), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008).

acetonitrile molecules is caused by weak intermolecular contacts between acetonitrile H atoms and adjacent fppy aldehyde carbonyl O atoms (C28—H28···O1) in addition to weak interactions between acetonitrile N atoms and adjacent DMSO H atoms (C25—H25*B*···N3). There are also C—H···O interactions between adjacent complexes, involving aromatic H atoms of one of the fppy ligands and methyl groups of the DMSO ligand with the sulfoxide O atom. Numerical details of all these interactions are collated in Table 1.

4. Database survey

A search of the Cambridge Structural Database (CSD, V5.38, update February 2017; Groom *et al.*, 2016) for related structures revealed that the di-μ-chlorido-bis{bis[4-(pyridin-2-yl)-benzaldehyde-κ^2C^2,N']iridium(III)} complex from which the title complex was derived, has been reported as a dichloromethane sesquisolvate (Bettington *et al.*, 2004).

5. Synthesis and crystallization

The parent compound, di-μ-chlorido-bis{bis[4-(pyridin-2-yl)-benzaldehyde-κ^2C^2,N']iridium(III), was synthesized utilizing a previously reported procedure (Bettington *et al.*, 2004).

For the synthesis of the title compound, di-μ-chlorido-bis{bis[4-(pyridin-2-yl)benzaldehyde-k$^2C^2$,N']iridium(III) (0.101 g, 0.077 mmol) was dissolved in DMSO (2 ml) with gentle heating over 5 min. After cooling to room temperature, acetonitrile (2 ml) was added. After 24 h, the resulting solid was collected by vacuum filtration to afford the title compound as an orange crystalline solid (0.043 g, 41.7%). Spectroscopic data: ^{1}H NMR (500 MHz, DMSO-d_6): δ 9.83 (*d*, 1H, J = 8.0 Hz), 9.61 (*s*, 1H), 9.55–9.53 (*m*, 2H), 8.42 (*d*, 1H, J = 8.0 Hz), 8.34 (*d*, 1H, J = 8.0 Hz), 8.20 (*t*, 1H, J = 7.5 Hz), 8.11 (*t*, 1H, J = 7.5 Hz), 8.01 (*d*, 1H, J = 7.5 Hz), 7.96 (*d*, 1H, J = 8.0 Hz), 7.69 (*t*, 1H, J = 6.5 Hz), 7.60 (*t*, 1H, J = 6.5 Hz), 7.40 (*d*, 1H, J = 8.0 Hz), 7.36 (*d*, 1H, J = 8.0 Hz), 6.71 (*s*, 1H), 6.10 (*s*, 1H) and ^{13}C NMR (500 MHz, DMSO-d_6): δ 193.6, 193.5, 166.1, 165.7, 153.1, 152.1, 151.7, 150.5, 149.9, 145.5, 140.4, 139.4, 136.6, 135.9, 131.2, 129.4, 126.4, 125.9, 125.7, 125.5, 125.2, 124.8, 122.4, 121.8, 72.3, 66.0, 60.8, 40.5, 40.3, 40.1, 40.0, 39.8, 39.6, 39.5, 15.7.

6. Refinement

Crystal data as well as data collection and structure refinement details are summarized in Table 2. The aldehyde hydrogen atoms were found in a difference-Fourier map and were refined freely. The remaining hydrogen atoms were included in calculated positions and refined with a riding model: C—H = 0.95-0.98 Å with $U_{\rm iso}$(H) = 1.5 $U_{\rm eq}$(C-methyl) and 1.2 $U_{\rm eq}$(C) for other H atoms.

Funding information

This work was supported by the Defense Threat Reduction Agency (DTRA) - Joint Science and Technology Transfer Office for Chemical and Biological Defense (MIPR No. HDTRA13964) and the Air Force Office of Scientific Research (AFOSR).

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Acta Cryst. (2017). E**73**, 1279–1281 Peloquin *et al.* • $[\mathrm{IrCl(C_{12}H_8NO)_2(C_2H_6OS)}]\cdot\mathrm{C_2H_3N}$ **1281**

supporting information

Acta Cryst. (2017). E**73**, 1279-1281   [https://doi.org/10.1107/S2056989017010945]

Crystal structure of chlorido(dimethyl sulfoxide-*κS*)bis[4-(pyridin-2-yl)benzaldehyde-κ^3C^2,*N*]iridium(III) acetonitrile monosolvate

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Computing details

Data collection: *APEX3* (Bruker, 2017); cell refinement: *SAINT* (Bruker, 2017); data reduction: *SAINT* (Bruker, 2017); program(s) used to solve structure: *SHELXS* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL2016* (Sheldrick, 2015).

Chlorido(dimethyl sulfoxide-*κS*)bis[4-(pyridin-2-yl)benzaldehyde-κ^2C^3,*N*]iridium(III) acetonitrile monosolvate

Crystal data

$[IrCl(C_{12}H_8NO)_2(C_2H_6OS)]\cdot C_2H_3N$
M_r = 711.22
Triclinic, $P\overline{1}$
a = 8.7837 (12) Å
b = 12.0910 (16) Å
c = 14.0097 (19) Å
α = 97.5367 (15)°
β = 105.1501 (14)°
γ = 109.3176 (14)°
V = 1316.1 (3) Å^3
Z = 2
$F(000)$ = 696
D_x = 1.795 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9979 reflections
θ = 2.6–30.0°
μ = 5.29 mm^{-1}
T = 100 K
Rectangular prism, orange
0.32 × 0.24 × 0.17 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ω Scans scans
Absorption correction: multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min} = 0.26, T_{max} = 0.47
28976 measured reflections
6983 independent reflections
6828 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 29.1°, θ_{min} = 1.8°
$h = -11\rightarrow11$
$k = -16\rightarrow16$
$l = -19\rightarrow19$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.037
S = 1.68
6983 reflections
345 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2)]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.003$

$\Delta\rho_{max} = 1.47$ e Å^{-3}
$\Delta\rho_{min} = -0.65$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	$U_{iso}*/U_{eq}$
C1	−0.0050 (3)	0.6613 (2)	0.33167 (17)	0.0243 (5)
H1	−0.088 (3)	0.596 (2)	0.278 (2)	0.042 (8)*
C2	0.1092 (2)	0.62505 (18)	0.40746 (15)	0.0157 (4)
H2	0.077 (3)	0.594 (2)	0.9857 (18)	0.028 (6)*
C3	0.2305 (2)	0.71022 (17)	0.49507 (14)	0.0134 (4)
H3	0.239758	0.790067	0.505177	0.016*
C4	0.3376 (2)	0.67614 (16)	0.56730 (14)	0.0100 (3)
C5	0.3222 (2)	0.55552 (16)	0.54791 (14)	0.0116 (4)
C6	0.2015 (2)	0.46989 (17)	0.46076 (14)	0.0151 (4)
H6	0.193066	0.390228	0.449892	0.018*
C7	0.0941 (2)	0.50534 (17)	0.39041 (15)	0.0164 (4)
H7	0.012541	0.449242	0.332285	0.02*
C8	0.6532 (2)	0.60005 (17)	0.78483 (14)	0.0134 (4)
H8	0.724573	0.664417	0.840195	0.016*
C9	0.6625 (2)	0.48877 (17)	0.78530 (15)	0.0167 (4)
H9	0.737233	0.47808	0.840651	0.02*
C10	0.5597 (3)	0.39315 (17)	0.70259 (15)	0.0175 (4)
H10	0.566006	0.317648	0.70063	0.021*
C11	0.4471 (2)	0.41157 (16)	0.62266 (15)	0.0153 (4)
H11	0.37664	0.348031	0.566469	0.018*
C12	0.4389 (2)	0.52483 (16)	0.62615 (14)	0.0112 (3)
C13	0.1550 (3)	0.57976 (18)	0.94959 (15)	0.0176 (4)
C14	0.1860 (2)	0.66267 (16)	0.88152 (14)	0.0128 (4)
C15	0.3053 (2)	0.66650 (16)	0.83096 (14)	0.0122 (4)
H15	0.363082	0.614479	0.838132	0.015*
C16	0.3375 (2)	0.74788 (16)	0.77005 (13)	0.0098 (3)
C17	0.2417 (2)	0.82202 (16)	0.75755 (14)	0.0108 (3)
C18	0.1194 (2)	0.81540 (17)	0.80579 (14)	0.0133 (4)
H18	0.055266	0.863072	0.795451	0.016*
C19	0.0948 (2)	0.73674 (16)	0.86940 (14)	0.0143 (4)
H19	0.016858	0.733882	0.903893	0.017*
C20	0.5027 (2)	1.00524 (16)	0.62983 (14)	0.0120 (4)
H20	0.605771	1.014028	0.61919	0.014*
C21	0.4188 (2)	1.07846 (16)	0.59468 (14)	0.0141 (4)
H21	0.464917	1.135452	0.560855	0.017*
C22	0.2647 (2)	1.06543 (17)	0.61075 (14)	0.0157 (4)

H22	0.204513	1.111646	0.585708	0.019*
C23	0.2021 (2)	0.98295 (17)	0.66440 (14)	0.0145 (4)
H23	0.100937	0.97487	0.67742	0.017*
C24	0.2915 (2)	0.91196 (16)	0.69888 (14)	0.0111 (3)
C25	0.6344 (2)	0.96111 (17)	0.94371 (14)	0.0157 (4)
H25A	0.559874	0.894382	0.96093	0.024*
H25B	0.570208	1.004318	0.911162	0.024*
H25C	0.722715	1.014181	1.004546	0.024*
C26	0.8560 (2)	1.04751 (17)	0.84339 (15)	0.0164 (4)
H26A	0.94507	1.092567	0.906542	0.025*
H26B	0.786226	1.092503	0.823195	0.025*
H26C	0.905534	1.033313	0.791846	0.025*
C27	0.5454 (3)	0.76301 (18)	0.12214 (16)	0.0216 (4)
C28	0.6709 (3)	0.7132 (2)	0.1106 (2)	0.0364 (6)
H28A	0.723039	0.747741	0.063586	0.055*
H28B	0.615895	0.62727	0.085237	0.055*
H28C	0.756838	0.731849	0.175519	0.055*
Cl1	0.74293 (5)	0.83320 (4)	0.62149 (3)	0.01155 (8)
Ir1	0.51788 (2)	0.78209 (2)	0.70247 (2)	0.00795 (2)
N1	0.54447 (18)	0.61957 (13)	0.70713 (11)	0.0097 (3)
N2	0.43895 (18)	0.92185 (13)	0.67888 (11)	0.0097 (3)
N3	0.4464 (3)	0.80168 (17)	0.13125 (15)	0.0286 (4)
O1	−0.0021 (2)	0.76266 (15)	0.33564 (13)	0.0390 (4)
O2	0.21023 (19)	0.50165 (13)	0.95953 (12)	0.0254 (3)
O3	0.84599 (17)	0.85806 (12)	0.92054 (10)	0.0171 (3)
S1	0.72772 (6)	0.90632 (4)	0.85936 (3)	0.01024 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0214 (11)	0.0248 (12)	0.0157 (11)	0.0071 (9)	−0.0064 (9)	−0.0016 (9)
C2	0.0133 (9)	0.0191 (10)	0.0105 (9)	0.0047 (8)	0.0002 (7)	0.0014 (8)
C3	0.0139 (9)	0.0122 (9)	0.0120 (9)	0.0044 (7)	0.0025 (7)	0.0009 (7)
C4	0.0090 (8)	0.0121 (8)	0.0086 (8)	0.0029 (7)	0.0042 (7)	0.0018 (7)
C5	0.0110 (8)	0.0134 (9)	0.0089 (9)	0.0030 (7)	0.0032 (7)	0.0018 (7)
C6	0.0161 (9)	0.0110 (9)	0.0128 (9)	0.0017 (7)	0.0024 (8)	−0.0008 (7)
C7	0.0147 (9)	0.0165 (10)	0.0096 (9)	0.0012 (8)	−0.0010 (7)	−0.0022 (7)
C8	0.0123 (9)	0.0137 (9)	0.0116 (9)	0.0046 (7)	0.0007 (7)	0.0018 (7)
C9	0.0192 (10)	0.0158 (10)	0.0149 (10)	0.0082 (8)	0.0020 (8)	0.0056 (8)
C10	0.0227 (10)	0.0124 (9)	0.0184 (10)	0.0075 (8)	0.0069 (8)	0.0050 (8)
C11	0.0191 (10)	0.0101 (9)	0.0127 (9)	0.0024 (7)	0.0040 (8)	0.0002 (7)
C12	0.0111 (8)	0.0125 (9)	0.0085 (9)	0.0029 (7)	0.0033 (7)	0.0011 (7)
C13	0.0199 (10)	0.0180 (10)	0.0151 (10)	0.0048 (8)	0.0089 (8)	0.0043 (8)
C14	0.0124 (9)	0.0130 (9)	0.0084 (9)	0.0012 (7)	0.0015 (7)	0.0007 (7)
C15	0.0112 (8)	0.0124 (9)	0.0098 (9)	0.0033 (7)	0.0007 (7)	0.0008 (7)
C16	0.0094 (8)	0.0086 (8)	0.0070 (8)	0.0032 (7)	−0.0019 (7)	−0.0025 (7)
C17	0.0088 (8)	0.0112 (8)	0.0080 (8)	0.0019 (7)	−0.0005 (7)	−0.0008 (7)
C18	0.0092 (8)	0.0154 (9)	0.0131 (9)	0.0052 (7)	0.0010 (7)	0.0000 (7)

C19	0.0106 (9)	0.0160 (9)	0.0133 (9)	0.0020 (7)	0.0044 (7)	0.0003 (7)
C20	0.0127 (9)	0.0114 (9)	0.0089 (9)	0.0024 (7)	0.0021 (7)	0.0011 (7)
C21	0.0194 (9)	0.0103 (9)	0.0099 (9)	0.0044 (7)	0.0023 (7)	0.0023 (7)
C22	0.0184 (10)	0.0141 (9)	0.0132 (9)	0.0093 (8)	−0.0008 (8)	0.0024 (8)
C23	0.0122 (9)	0.0161 (9)	0.0135 (9)	0.0063 (7)	0.0016 (7)	0.0009 (8)
C24	0.0111 (8)	0.0103 (8)	0.0083 (9)	0.0031 (7)	0.0005 (7)	−0.0014 (7)
C25	0.0198 (10)	0.0157 (9)	0.0099 (9)	0.0069 (8)	0.0044 (8)	−0.0015 (7)
C26	0.0152 (9)	0.0126 (9)	0.0154 (10)	0.0006 (7)	0.0029 (8)	0.0007 (8)
C27	0.0265 (11)	0.0167 (10)	0.0151 (10)	0.0054 (9)	−0.0007 (9)	0.0057 (8)
C28	0.0377 (14)	0.0438 (15)	0.0351 (15)	0.0235 (12)	0.0108 (12)	0.0149 (12)
Cl1	0.01124 (19)	0.0134 (2)	0.0103 (2)	0.00477 (16)	0.00389 (16)	0.00282 (16)
Ir1	0.00779 (4)	0.00810 (4)	0.00644 (4)	0.00263 (3)	0.00083 (3)	0.00086 (3)
N1	0.0098 (7)	0.0095 (7)	0.0091 (7)	0.0035 (6)	0.0024 (6)	0.0017 (6)
N2	0.0107 (7)	0.0096 (7)	0.0065 (7)	0.0032 (6)	0.0008 (6)	0.0004 (6)
N3	0.0378 (11)	0.0250 (10)	0.0226 (10)	0.0156 (9)	0.0042 (9)	0.0067 (8)
O1	0.0454 (11)	0.0286 (9)	0.0291 (10)	0.0197 (8)	−0.0143 (8)	0.0008 (8)
O2	0.0343 (9)	0.0235 (8)	0.0257 (9)	0.0135 (7)	0.0150 (7)	0.0131 (7)
O3	0.0172 (7)	0.0168 (7)	0.0129 (7)	0.0100 (6)	−0.0048 (6)	−0.0009 (6)
S1	0.0108 (2)	0.0099 (2)	0.0079 (2)	0.00406 (16)	0.00035 (16)	0.00033 (16)

Geometric parameters (Å, º)

C1—O1	1.211 (3)	C16—C17	1.416 (2)
C1—C2	1.477 (3)	C16—Ir1	2.0077 (18)
C2—C7	1.391 (3)	C17—C18	1.398 (2)
C2—C3	1.400 (3)	C17—C24	1.469 (2)
C3—C4	1.396 (3)	C18—C19	1.390 (3)
C4—C5	1.402 (3)	C20—N2	1.346 (2)
C4—Ir1	2.0466 (18)	C20—C21	1.388 (3)
C5—C6	1.397 (3)	C21—C22	1.391 (3)
C5—C12	1.470 (3)	C22—C23	1.383 (3)
C6—C7	1.392 (3)	C23—C24	1.394 (3)
C8—N1	1.351 (2)	C24—N2	1.366 (2)
C8—C9	1.376 (3)	C25—S1	1.7799 (19)
C9—C10	1.381 (3)	C26—S1	1.7870 (19)
C10—C11	1.384 (3)	C27—N3	1.141 (3)
C11—C12	1.390 (3)	C27—C28	1.453 (3)
C12—N1	1.366 (2)	Cl1—Ir1	2.4748 (5)
C13—O2	1.204 (2)	Ir1—N2	2.0609 (15)
C13—C14	1.481 (3)	Ir1—N1	2.0614 (15)
C14—C19	1.384 (3)	Ir1—S1	2.3810 (5)
C14—C15	1.402 (2)	O3—S1	1.4903 (13)
C15—C16	1.392 (2)		
O1—C1—C2	125.8 (2)	C20—C21—C22	119.06 (17)
C7—C2—C3	120.72 (18)	C23—C22—C21	119.21 (17)
C7—C2—C1	119.00 (18)	C22—C23—C24	119.65 (17)
C3—C2—C1	120.28 (18)	N2—C24—C23	120.64 (16)

C4—C3—C2	120.47 (18)	N2—C24—C17	113.70 (15)
C3—C4—C5	117.90 (17)	C23—C24—C17	125.66 (16)
C3—C4—Ir1	127.61 (14)	N3—C27—C28	179.7 (2)
C5—C4—Ir1	114.48 (13)	C16—Ir1—C4	89.71 (7)
C6—C5—C4	122.04 (17)	C16—Ir1—N2	80.48 (6)
C6—C5—C12	122.36 (17)	C4—Ir1—N2	89.53 (7)
C4—C5—C12	115.59 (16)	C16—Ir1—N1	93.83 (6)
C7—C6—C5	119.15 (18)	C4—Ir1—N1	79.63 (7)
C2—C7—C6	119.70 (18)	N2—Ir1—N1	167.83 (6)
N1—C8—C9	122.61 (18)	C16—Ir1—S1	90.41 (5)
C8—C9—C10	119.19 (19)	C4—Ir1—S1	179.68 (5)
C9—C10—C11	118.86 (18)	N2—Ir1—S1	90.19 (4)
C10—C11—C12	120.15 (18)	N1—Ir1—S1	100.65 (4)
N1—C12—C11	120.48 (17)	C16—Ir1—Cl1	177.65 (5)
N1—C12—C5	113.96 (16)	C4—Ir1—Cl1	91.58 (5)
C11—C12—C5	125.56 (17)	N2—Ir1—Cl1	97.56 (4)
O2—C13—C14	126.05 (18)	N1—Ir1—Cl1	88.33 (4)
C19—C14—C15	120.78 (17)	S1—Ir1—Cl1	88.295 (18)
C19—C14—C13	118.36 (17)	C8—N1—C12	118.67 (16)
C15—C14—C13	120.86 (17)	C8—N1—Ir1	124.98 (12)
C16—C15—C14	120.26 (17)	C12—N1—Ir1	116.32 (12)
C15—C16—C17	118.19 (16)	C20—N2—C24	119.49 (15)
C15—C16—Ir1	127.48 (13)	C20—N2—Ir1	124.76 (12)
C17—C16—Ir1	114.21 (13)	C24—N2—Ir1	114.59 (11)
C18—C17—C16	121.29 (17)	O3—S1—C25	106.03 (9)
C18—C17—C24	123.30 (17)	O3—S1—C26	107.19 (9)
C16—C17—C24	115.18 (15)	C25—S1—C26	98.72 (9)
C19—C18—C17	119.24 (17)	O3—S1—Ir1	119.58 (6)
C14—C19—C18	120.16 (17)	C25—S1—Ir1	111.64 (7)
N2—C20—C21	121.84 (17)	C26—S1—Ir1	111.52 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C19—H19···O3^{i}	0.93	2.48	3.179 (3)	132
C25—H25*B*···N3^{ii}	0.96	2.53	3.403 (3)	150
C26—H26*A*···O3^{iii}	0.96	2.48	3.406 (2)	161
C28—H28*C*···O1^{iv}	0.96	2.54	3.490 (3)	173

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*+1, −*y*+2, −*z*+1; (iii) −*x*+2, −*y*+2, −*z*+2; (iv) *x*+1, *y*, *z*.