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(N,N'-Diethyldithiocarbamato-κ^2S,S')-bis[2-(2-pyridyl)phenyl-κ^2C^1,N]-iridium(III)

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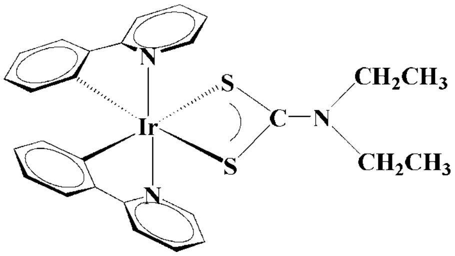
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.023; wR factor = 0.071; data-to-parameter ratio = 18.6.

In the title compound, $[Ir(C_{11}H_8N)_2(C_5H_{10}NS_2)]$, the Ir center has a distorted octahedral environment. The N donors of the two chelating 2-(2-pyridyl)phenyl ligands are in *trans* positions with respect to each other and the two C atoms are in a *cis* configuration. The packing is partially facilitated by C—H$\cdots\pi$ interactions between aromatic rings in neighboring molecules, connecting the molecules into infinite chains along the c axis of the unit cell. These chains are in turn connected by C—H$\cdots\pi$ interactions between neighboring chains. A crystallographic twofold rotation axis passes through Ir and C,N of the dithiocarbamate ligand.

Related literature

For related literature, see: Baldo *et al.* (1998); Garces *et al.* (1993); Lamansky *et al.* (2001); Sprouse et al. (1984).



Experimental

Crystal data

$[Ir(C_{11}H_8N)_2(C_5H_{10}NS_2)]$
M_r = 648.83
Monoclinic, $C2/c$
a = 16.401 (3) Å
b = 11.436 (2) Å
c = 13.540 (3) Å
β = 99.00 (3)°
V = 2508.2 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 5.51 mm^{-1}
T = 293 (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.576, T_{max} = 0.582
2852 measured reflections
2852 independent reflections
2597 reflections with $I > 2\sigma(I)$
R_{int} = 0.000

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.071
S = 1.15
2852 reflections
153 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.87 e Å^{-3}
$\Delta\rho_{min}$ = −1.12 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ir1—C11	2.015 (4)	Ir1—S1	2.4792 (11)
Ir1—N1	2.045 (4)		
C11^{i}—Ir1—C11	90.6 (2)	N1—Ir1—S1	97.86 (10)
N1—Ir1—N1^{i}	173.25 (17)	N1^{i}—Ir1—S1	87.65 (9)
C11^{i}—Ir1—S1	170.21 (11)	S1—Ir1—S1^{i}	71.12 (5)
C11—Ir1—S1	99.15 (12)		

Symmetry code: (i) $-x, y, -z + \frac{1}{2}$.

Table 2
Hydrogen-bond geometry (Å, °).

$Cg1$ and $Cg2$ are the centroids of the C6–C11 and N1/C1–C5 rings, respectively.

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C4—H4$\cdots Cg1^{ii}$	0.93	2.85	3.610 (6)	140
C8—H8$\cdots Cg2^{iii}$	0.93	3.00	3.897 (7)	163

Symmetry codes: (ii) $x + \frac{1}{2}, y + \frac{1}{2}, z$; (iii) $-x, -y - 1, -z$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: ZL2022).

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supplementary materials

Acta Cryst. (2007). E**63**, m2078 [**doi:10.1107/S1600536807032126**]

(*N*,*N*'-Diethyldithiocarbamato-κ^2*S*,*S*')bis[2-(2-pyridyl)phenyl-κ^2*C*^{1},*N*]iridium(III)

L.-Q. Chen

Comment

Organic light-emitting diodes (OLEDs) have been actively investigated due to their potential applications in flat panel displays and light-emitting devices. Most recently, heavy metal complexes in OLEDs have attracted much attention as efficient phosphors because they can harvest both singlet and triplet excited states, and thus the OLEDs internal efficiency can theoretically reach 100% (Lamansky *et al.*, 2001). Especially iridium (III) complexes with cyclometalated ligands show intense phosphorescence at room temperature and this behavior makes them very promising phosphor dyes in OLEDs (Baldo *et al.*, 1998 & Lamansky *et al.*, 2001). Also, metal complexes containing dithiolate ligands have been extensively studied. However, only relatively few iridium (III) dithiolate complexes have been described. The title compound, which emits green luminescence in both solid state and organic solution upon irradiation by UV-light at ambient temperature, may plays a very important role as a potential electrophosphorescent material.

In the crystal structure of the title molecule, the Ir center resides in a distorted octahedral environment. The nitrogen donors of the the two chelating 2-phenylpyridinato ligands are in *trans* posistion to each other, the two carbon atoms are in a *cis* configuration (Scheme 1). As expected, the Ir—C bonds (2.015 (4) Å) are shorter than the Ir—N bond distances (2.045 (4) Å). These values are very similar to those in similar complexes such as (ppy)$_2$Ir(acac) (ppy: 2-phenylpyridine; acac: actylacetone)(Ir—C: 2.020 (2) Å; Ir—N: 2.090 (10) Å) (Garces *et al.*, 1993). The similarity of the S—C bond lengths in the *N*,*N*'-diethyldithiocarbamate (Et$_2$dtc) ligand indicates that the charge is delocalized over both sulfur atoms. The Et$_2$dtc chelate angle (S1—Ir1—S1a) is 71.12 (5)°, and the phenyl and metalated pyridine rings in the same ppy ligand are coplanar (the dihedral angle between the two planes is 0.3 (1)°). Selected important bond distances and angles are given in the selected geomtetric parameters table.

The packing of compound (I) is partially facilitated by C—H···π interactions between aromatic rings in neighboring molecules, the two most prominent such interactions are given in the hydrogen bonding table (*Cg*1 represents the centroid of ring C6/C7/C8/C9/C10/C11, *Cg*2 that of N1/C1/C2/C3/C4/C5). The first of these interactions, which acts in centrosymmetric pairs between each two molecules, connects the molecules to infinite chains along the *c* axis of the unit cell. The second slightly weaker type of C—H···π interaction connects these chains with each other (Figures 2 and 3).

Experimental

Iridium trichloride hydrate and 2-phenylpyridine were purchased and used without further purification. The synthesis of the target product involves two steps. First, iridium trichloride hydrate (0.352 g, 1.0 mmol) was combined with 2.5 equiv of the cyclometalating ligand, 2-phenylpyridine (0.385 g, 2.5 mmol), was dissolved in a mixture of 2-ethoxyethanol (30 ml) and water (10 ml), and then refluxed for 24 h. The solution was cooled to room temperature, and the yellow precipitate was collected on a glass filter frit. After drying, the crude product was directly used for the next step without further purification (Watts *et al.*, 1984). In the second step, the product (0.075 mmol), sodium *N*,*N*'-diethyldithio-carbamate (NaEt$_2$dtc) (0.25 mmol) and anhydrous sodium carbonate (Na$_2$CO$_3$, 1.0 mmol) were dissolved in 2-ethoxyethanol (10 ml). The mixture was refluxed under argon for 18 h. After cooling to room temperature, a small quantity of water was added. The resulting red precipitate was collected by filtration, washed with water, ethanol and hexane, and dried in vacuum. The crude product was purified by column chromatography on silica gel with CH_2Cl_2/petroleum ether (1:3) as the eluent. The residue was dried under vacuum and recrystallized from dichloromethane/hexane (1:1, *v*/*v*). Yield: 0.215 g (65.2%), ^{1}H NMR ($CDCl_3$, 300 MHz, p.p.m.) 1.20–1.25 (t, J = 7.5 Hz, 6H), 3.46–3.53 (m, 2H), 3.73–3.80 (m, 2H), 6.28 (d, J = 7.8 Hz, 2H), 6.60 (dd, J = 7.2 Hz, 2H), 6.76 (dd, J = 8.1 Hz, 2H), 7.14–7.21 (m, 2H), 7.50 (d, J = 8.4 Hz, 2H) 7.66 (dd, J = 6.9 Hz, 2H) 7.81 (d, J = 7.2 Hz, 2H) 9.57 (d, J = 8.7 Hz, 2H). Calcd for $C_{27}H_{26}N_3S_2Ir$: C, 49.98; H, 4.04; N, 6.48%, Found: C, 50.23; H, 4.10; N, 6.21%. MS (FAB): m/e, 649 (M^+).

Refinement

All H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances in the range 0.93–0.98 Å, and with $U_{\rm iso}$(H) = 1.2U $_{\rm eq}$ for aryl H atoms and 1.5$U_{\rm eq}$ for the methyl H atoms. Methyl H atoms were allowed to rotate to best fit the experimental electron density.

Figures

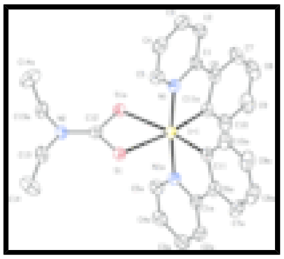

Fig. 1. The structure of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level (−*x*, *y*, 0.5 − *z*).

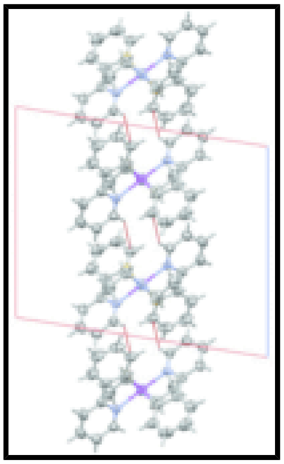

Fig. 2. Packing Diagram of (I), view down the *b* axis showing the infinite chains created by the C—H···π interactions between C4—H4 and the ring C6/C7/C8/C9/C10/C11.

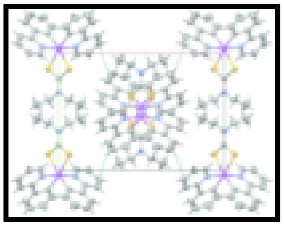

Fig. 3. Packing Diagram of (I), view down the *c* axis along the infinite chains shown in Figure 2. Red dashed lines: C—H···π interactions of C4—H4 to ring C6/C7/C8/C9/C10/C11 forming the infinite chains. Blue: C8—H8 to ring N1/C1/C2/C3/C4/C5 connecting these chains.

(*N*,*N*'-Diethyldithiocarbamato-κ^2*S*,*S*')bis[2-(2-pyridyl)phenyl- κ^2*C*^{1},*N*]iridium(III)

Crystal data

$[Ir(C_{11}H_8N)_2(C_5H_{10}NS_2)]$

$M_r = 648.83$

Monoclinic, $C2/c$

Hall symbol: -C 2yc

$a = 16.401$ (3) Å

$b = 11.436$ (2) Å

$c = 13.540$ (3) Å

$\beta = 99.00$ (3)°

$V = 2508.2$ (9) Å^3

$Z = 4$

$F_{000} = 1272$

$D_x = 1.718$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å

Cell parameters from 2854 reflections

$\theta = 4$–27.5°

$\mu = 5.51$ mm^{-1}

$T = 293$ (2) K

Block, red

0.10 × 0.10 × 0.10 mm

Data collection

Siemens SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 293(2)$ K

φ and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{min} = 0.576$, $T_{max} = 0.582$

2852 measured reflections

2852 independent reflections

2597 reflections with $I > 2\sigma(I)$

$R_{int} = 0.0000$

$\theta_{max} = 27.4$°

$\theta_{min} = 2.2$°

$h = 0 \rightarrow 21$

$k = 0 \rightarrow 14$

$l = -17 \rightarrow 17$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.023$

$wR(F^2) = 0.071$

$S = 1.15$

2852 reflections

153 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0376P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.87$ e Å^{-3}

$\Delta\rho_{min} = -1.12$ e Å^{-3}

Extinction correction: SHELXL97 (Sheldrick, 1997a), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0046 (2)

Special details

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

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

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

	x	y	z	U_{iso}*/U_{eq}
C1	−0.1615 (2)	−0.1270 (4)	0.1595 (3)	0.0431 (9)
C2	−0.2324 (3)	−0.1397 (4)	0.0889 (4)	0.0536 (11)
H2	−0.2740	−0.1899	0.1020	0.064*
C3	−0.2418 (3)	−0.0792 (5)	0.0005 (4)	0.0594 (12)
H3	−0.2889	−0.0891	−0.0469	0.071*
C4	−0.1801 (3)	−0.0031 (5)	−0.0171 (4)	0.0566 (11)
H4	−0.1851	0.0395	−0.0763	0.068*
C5	−0.1117 (3)	0.0082 (5)	0.0544 (3)	0.0476 (10)
H5	−0.0704	0.0597	0.0425	0.057*
C6	0.1429 (3)	−0.1884 (4)	0.2456 (3)	0.0459 (9)
C7	0.1972 (3)	−0.2661 (4)	0.2101 (4)	0.0649 (14)
H7	0.2485	−0.2814	0.2479	0.078*
C8	0.1746 (4)	−0.3200 (5)	0.1191 (5)	0.0761 (16)
H8	0.2115	−0.3693	0.0940	0.091*
C9	0.0977 (4)	−0.3010 (5)	0.0653 (4)	0.0711 (15)
H9	0.0821	−0.3398	0.0050	0.085*
C10	0.0428 (3)	−0.2244 (4)	0.1000 (3)	0.0557 (11)
H10	−0.0091	−0.2126	0.0627	0.067*
C11	0.0647 (3)	−0.1648 (3)	0.1901 (3)	0.0405 (8)
C12	0.0000	0.2174 (5)	0.2500	0.0392 (12)
C13	0.0614 (3)	0.4009 (4)	0.2065 (4)	0.0583 (12)
H13A	0.0350	0.4686	0.1720	0.070*
H13B	0.0837	0.3532	0.1578	0.070*
C14	0.1303 (5)	0.4405 (6)	0.2859 (7)	0.095 (2)
H14A	0.1091	0.4938	0.3304	0.143*
H14B	0.1719	0.4790	0.2551	0.143*
H14C	0.1541	0.3739	0.3230	0.143*
Ir1	0.0000	−0.040880 (17)	0.2500	0.03458 (10)
N1	−0.1011 (2)	−0.0514 (3)	0.1408 (3)	0.0382 (7)
N2	0.0000	0.3332 (4)	0.2500	0.0454 (11)
S1	0.06343 (6)	0.13548 (9)	0.18733 (8)	0.0423 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.045 (2)	0.0360 (19)	0.050 (2)	−0.0042 (17)	0.0123 (16)	−0.0108 (19)
C2	0.050 (2)	0.047 (2)	0.063 (3)	−0.0046 (19)	0.007 (2)	−0.015 (2)
C3	0.057 (3)	0.059 (3)	0.058 (3)	0.009 (2)	−0.005 (2)	−0.014 (3)
C4	0.062 (3)	0.059 (3)	0.048 (3)	0.014 (2)	0.004 (2)	0.000 (2)
C5	0.050 (2)	0.051 (2)	0.042 (2)	0.005 (2)	0.0099 (18)	0.005 (2)
C6	0.056 (2)	0.036 (2)	0.048 (2)	0.0074 (18)	0.0196 (18)	0.0059 (19)
C7	0.069 (3)	0.053 (3)	0.077 (4)	0.024 (2)	0.022 (3)	0.005 (3)
C8	0.096 (4)	0.057 (3)	0.082 (4)	0.029 (3)	0.036 (3)	−0.008 (3)
C9	0.109 (4)	0.054 (3)	0.055 (3)	0.013 (3)	0.027 (3)	−0.014 (3)
C10	0.074 (3)	0.046 (2)	0.050 (3)	0.005 (2)	0.018 (2)	−0.002 (2)
C11	0.050 (2)	0.0335 (19)	0.040 (2)	0.0012 (16)	0.0147 (16)	0.0005 (17)
C12	0.032 (2)	0.045 (3)	0.040 (3)	0.000	0.005 (2)	0.000
C13	0.068 (3)	0.040 (2)	0.068 (3)	−0.009 (2)	0.015 (2)	0.006 (2)
C14	0.080 (4)	0.102 (5)	0.104 (6)	−0.041 (4)	0.014 (4)	−0.004 (4)
Ir1	0.03838 (14)	0.03183 (13)	0.03526 (14)	0.000	0.01116 (8)	0.000
N1	0.0421 (17)	0.0381 (17)	0.0355 (17)	0.0013 (13)	0.0092 (13)	−0.0024 (13)
N2	0.045 (3)	0.034 (2)	0.057 (3)	0.000	0.011 (2)	0.000
S1	0.0413 (5)	0.0386 (5)	0.0504 (6)	−0.0006 (4)	0.0180 (4)	0.0012 (5)

Geometric parameters (Å, °)

C1—N1	1.367 (5)	C10—C11	1.394 (6)
C1—C2	1.393 (6)	C10—H10	0.9300
C1—C6^{i}	1.454 (6)	C11—Ir1	2.015 (4)
C2—C3	1.370 (7)	C12—N2	1.324 (8)
C2—H2	0.9300	C12—S1^{i}	1.719 (3)
C3—C4	1.384 (9)	C12—S1	1.719 (3)
C3—H3	0.9300	C13—N2	1.465 (5)
C4—C5	1.369 (7)	C13—C14	1.504 (9)
C4—H4	0.9300	C13—H13A	0.9700
C5—N1	1.342 (6)	C13—H13B	0.9700
C5—H5	0.9300	C14—H14A	0.9600
C6—C7	1.395 (6)	C14—H14B	0.9600
C6—C11	1.408 (6)	C14—H14C	0.9600
C6—C1^{i}	1.454 (6)	Ir1—C11^{i}	2.015 (4)
C7—C8	1.376 (8)	Ir1—N1	2.045 (4)
C7—H7	0.9300	Ir1—N1^{i}	2.045 (4)
C8—C9	1.371 (8)	Ir1—S1	2.4792 (11)
C8—H8	0.9300	Ir1—S1^{i}	2.4792 (11)
C9—C10	1.389 (7)	N2—C13^{i}	1.465 (5)
C9—H9	0.9300		
N1—C1—C2	119.3 (4)	S1^{i}—C12—S1	114.0 (3)
N1—C1—C6^{i}	114.3 (4)	N2—C13—C14	111.0 (5)

C2—C1—C6^{i}	126.4 (4)	N2—C13—H13A	109.4
C3—C2—C1	121.0 (4)	C14—C13—H13A	109.4
C3—C2—H2	119.5	N2—C13—H13B	109.4
C1—C2—H2	119.5	C14—C13—H13B	109.4
C2—C3—C4	118.9 (4)	H13A—C13—H13B	108.0
C2—C3—H3	120.6	C13—C14—H14A	109.5
C4—C3—H3	120.6	C13—C14—H14B	109.5
C5—C4—C3	118.6 (5)	H14A—C14—H14B	109.5
C5—C4—H4	120.7	C13—C14—H14C	109.5
C3—C4—H4	120.7	H14A—C14—H14C	109.5
N1—C5—C4	123.3 (5)	H14B—C14—H14C	109.5
N1—C5—H5	118.4	C11^{i}—Ir1—C11	90.6 (2)
C4—C5—H5	118.4	C11^{i}—Ir1—N1	80.27 (16)
C7—C6—C11	121.0 (4)	C11—Ir1—N1	94.94 (15)
C7—C6—C1^{i}	123.7 (4)	C11^{i}—Ir1—N1^{i}	94.94 (15)
C11—C6—C1^{i}	115.3 (3)	C11—Ir1—N1^{i}	80.27 (16)
C8—C7—C6	119.8 (5)	N1—Ir1—N1^{i}	173.25 (17)
C8—C7—H7	120.1	C11^{i}—Ir1—S1	170.21 (11)
C6—C7—H7	120.1	C11—Ir1—S1	99.15 (12)
C9—C8—C7	120.1 (5)	N1—Ir1—S1	97.86 (10)
C9—C8—H8	120.0	N1^{i}—Ir1—S1	87.65 (9)
C7—C8—H8	120.0	C11^{i}—Ir1—S1^{i}	99.15 (12)
C8—C9—C10	120.7 (5)	C11—Ir1—S1^{i}	170.21 (11)
C8—C9—H9	119.7	N1—Ir1—S1^{i}	87.65 (9)
C10—C9—H9	119.6	N1^{i}—Ir1—S1^{i}	97.86 (10)
C9—C10—C11	120.9 (5)	S1—Ir1—S1^{i}	71.12 (5)
C9—C10—H10	119.6	C5—N1—C1	119.0 (4)
C11—C10—H10	119.6	C5—N1—Ir1	125.4 (3)
C10—C11—C6	117.5 (4)	C1—N1—Ir1	115.6 (3)
C10—C11—Ir1	128.1 (3)	C12—N2—C13	121.9 (3)
C6—C11—Ir1	114.4 (3)	C12—N2—C13^{i}	121.9 (3)
N2—C12—S1^{i}	123.02 (17)	C13—N2—C13^{i}	116.2 (5)
N2—C12—S1	123.02 (17)	C12—S1—Ir1	87.46 (17)
N1—C1—C2—C3	1.2 (7)	C4—C5—N1—Ir1	179.1 (4)
C6^{i}—C1—C2—C3	−178.0 (4)	C2—C1—N1—C5	−0.4 (6)
C1—C2—C3—C4	−1.2 (7)	C6^{i}—C1—N1—C5	178.9 (4)
C2—C3—C4—C5	0.5 (8)	C2—C1—N1—Ir1	−179.9 (3)
C3—C4—C5—N1	0.3 (8)	C6^{i}—C1—N1—Ir1	−0.5 (4)
C11—C6—C7—C8	0.6 (7)	C11^{i}—Ir1—N1—C5	−177.0 (4)
C1^{i}—C6—C7—C8	−179.7 (5)	C11—Ir1—N1—C5	−87.2 (4)
C6—C7—C8—C9	−2.6 (9)	S1—Ir1—N1—C5	12.7 (4)
C7—C8—C9—C10	2.2 (9)	S1^{i}—Ir1—N1—C5	83.3 (3)
C8—C9—C10—C11	0.2 (8)	C11^{i}—Ir1—N1—C1	2.4 (3)
C9—C10—C11—C6	−2.1 (6)	C11—Ir1—N1—C1	92.2 (3)

C9—C10—C11—Ir1	174.7 (4)	S1—Ir1—N1—C1	−167.8 (3)
C7—C6—C11—C10	1.7 (6)	S1^{i}—Ir1—N1—C1	−97.3 (3)
C1^{i}—C6—C11—C10	−178.0 (4)	S1^{i}—C12—N2—C13	172.4 (3)
C7—C6—C11—Ir1	−175.5 (3)	S1—C12—N2—C13	−7.6 (3)
C1^{i}—C6—C11—Ir1	4.8 (5)	S1^{i}—C12—N2—C13^{i}	−7.6 (3)
C10—C11—Ir1—C11^{i}	84.4 (4)	S1—C12—N2—C13^{i}	172.4 (3)
C6—C11—Ir1—C11^{i}	−98.8 (3)	C14—C13—N2—C12	−98.1 (5)
C10—C11—Ir1—N1	4.1 (4)	C14—C13—N2—C13^{i}	81.9 (5)
C6—C11—Ir1—N1	−179.1 (3)	N2—C12—S1—Ir1	180.0
C10—C11—Ir1—N1^{i}	179.3 (4)	S1^{i}—C12—S1—Ir1	0.0
C6—C11—Ir1—N1^{i}	−3.9 (3)	C11—Ir1—S1—C12	−178.88 (12)
C10—C11—Ir1—S1	−94.7 (4)	N1—Ir1—S1—C12	84.78 (10)
C6—C11—Ir1—S1	82.1 (3)	N1^{i}—Ir1—S1—C12	−99.14 (10)
C4—C5—N1—C1	−0.3 (7)	S1^{i}—Ir1—S1—C12	0.0

Symmetry codes: (i) $-x, y, -z+1/2$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···Cg1^{ii}	0.93	2.85	3.610 (6)	140
C8—H8···Cg2^{iii}	0.93	3.00	3.897 (7)	163

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

Fig. 1

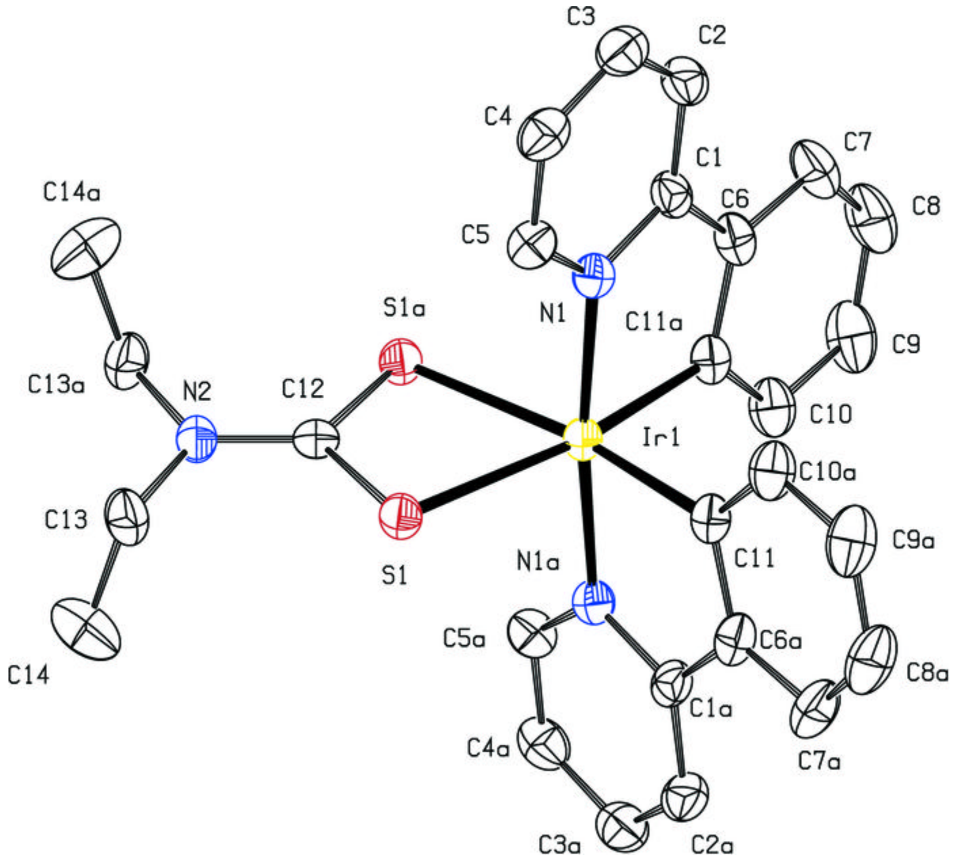
C3
C2
C4
C1
C7
C14a
C6
C8
C5
S1a
N1
C11a
C9
C13a
N2
C12
C10
Ir1
C10a
C13
C9a
C11
S1
N1a
C5a
C6a
C14
C8a
C1a
C4a
C7a
C3a
C2a

Fig. 2

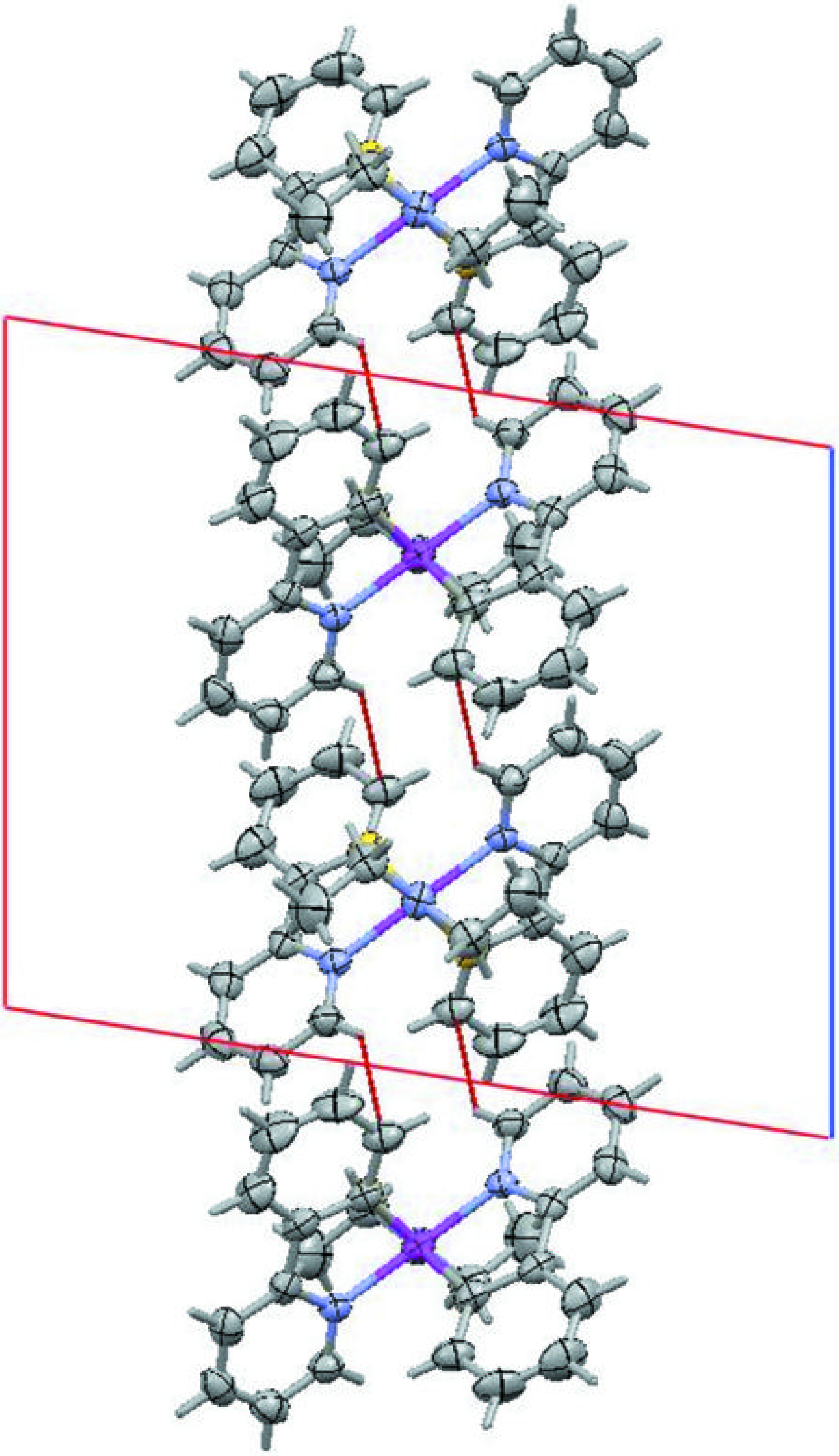

Fig. 3