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Chlorobis[2-(2-pyridyl)phenyl-κ^2N,C^1](triphenylphosphine-κP)iridium(III) dichloromethane sesquisolvate

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In the title compound, $[Ir(C_{11}H_8N)_2Cl(C_{18}H_{15}P)]\cdot1.5CH_2Cl_2$, the Ir^{III} atom is octahedrally coordinated by one Cl atom, one triphenylphosphine P atom and two *N,C*-bidentate 2-phenylpyridine (ppy) ligands. The crystal structure contains three dichloromethane solvent molecules for every two complex molecules.

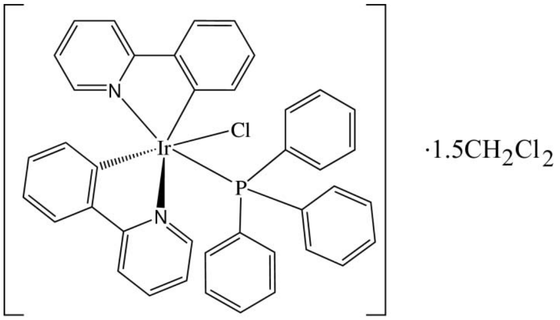
Key indicators

Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.013 Å
Disorder in solvent or counterion
R factor = 0.051
wR factor = 0.120
Data-to-parameter ratio = 14.7

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

Iridium(III) complexes have attracted considerable attention because of their applications as light-emitting diodes (Baldo *et al.*, 1998; Gong *et al.*, 2003; He *et al.*, 2004). The emission colour can be tuned by using ancillary ligands (Youshikawa *et al.*, 2004), because the ligand can affect the HOMO–LUMO energy gap (HUMO is the highest occupied molecular orbital and LUMO is the lowest unoccupied molecular orbital). In a number of previous reports of these types of compounds (Lamansky *et al.*, 2001; Duan *et al.*, 2003), 2,4-pentanedione (acac) was used as the ancillary ligand. We report here the use of triphenylphosphine in this role, which reacted with the dimer $Ir_2(ppy)_2Cl_2$ (Nonoyama, 1974) leading to the title compound, (I) (Fig. 1).



(I)

In (I), the Ir atom is coordinated by one Cl atom, one triphenylphosphine ligand and two *N,C*-bidentate 2-phenylpyridine (ppy) ligands. The two Ir—C(ppy) bond lengths (Table 1) are slightly different, perhaps because of steric hindrance from the other ligands. The bond angles about atom Ir1 (Table 1) do not indicate substantial distortion from octahedral regularity. For the two ppy units, the bonded N atoms (N1 and N2) are *trans* and the bonded C atoms (C29 and C40) are *cis* with respect to Ir1. The crystal packing in (I) is shown in Fig. 2.

Experimental

The reaction was performed under a nitrogen atmosphere and analytical grade solvents were used after further purification. At room temperature, 0.08 mmol $Ir_2(ppy)_2Cl_2$ (Nonoyama, 1974) was mixed with 0.16 mmol triphenylphosphine in dichloromethane (30 ml). The mixture was stirred for 10 h and filtered. Upon removal of the solvent by rotary evaporation, crude (I) was obtained as a yellow solid. The product was purified by passing through a column of silica using ethyl acetate/petroleum ether (1:1 *v*/*v*) as eluent. Crystals suitable for X-ray characterization were obtained by diffusing petroleum ether into a dichloromethane solution of (I).

Crystal data

$[Ir(C_{11}H_8N)_2Cl(C_{18}H_{15}P)]\cdot 1.5CH_2Cl_2$
$M_r = 925.68$
Monoclinic, $P2_1/c$
$a = 10.128$ (2) Å
$b = 15.038$ (3) Å
$c = 24.586$ (5) Å
$\beta = 99.70$ (3)°
$V = 3691.0$ (13) Å^3
$Z = 4$

$D_x = 1.666$ Mg m$^{-3$}
Mo $K\alpha$ radiation
Cell parameters from 23 091 reflections
$\theta = 2.5$–25.0°
$\mu = 3.98$ mm^{-1}
$T = 193$ (2) K
Block, colorless
0.50 × 0.20 × 0.10 mm

Data collection

Rigaku R-AXIS RAPID IP diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{min} = 0.241$, $T_{max} = 0.671$
23 091 measured reflections

6481 independent reflections
4616 reflections with $I > 2\sigma(I)$
$R_{int} = 0.087$
$\theta_{max} = 25.0°$
$h = -12 \rightarrow 12$
$k = -17 \rightarrow 17$
$l = -29 \rightarrow 29$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.051$
$wR(F^2) = 0.120$
$S = 0.96$
6481 reflections
442 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.004$
$\Delta\rho_{max} = 2.11$ e Å^{-3}
$\Delta\rho_{min} = -2.76$ e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0031 (2)

Table 1
Selected geometric parameters (Å, °).

Ir1—C40	2.024 (7)	Ir1—N2	2.044 (6)
Ir1—C29	2.031 (8)	Ir1—P4	2.426 (2)
Ir1—N1	2.043 (6)	Ir1—Cl1	2.5028 (19)
C40—Ir1—C29	88.1 (3)	N1—Ir1—P4	98.41 (19)
C40—Ir1—N1	94.2 (3)	N2—Ir1—P4	89.64 (18)
C29—Ir1—N1	80.5 (3)	C40—Ir1—Cl1	170.3 (2)
C40—Ir1—N2	79.9 (3)	C29—Ir1—Cl1	83.9 (2)
C29—Ir1—N2	92.0 (3)	N1—Ir1—Cl1	89.93 (16)
N1—Ir1—N2	170.7 (2)	N2—Ir1—Cl1	94.81 (18)
C40—Ir1—P4	98.2 (2)	P4—Ir1—Cl1	89.84 (7)
C29—Ir1—P4	173.7 (2)		

All H atoms were placed in geometrically idealized positions and refined as riding, with C—H distances in the range 0.95–1.00 Å. The constraint $U_{iso}(H) = 1.2U_{eq}$(carrier) or $1.5U_{eq}$(carrier) was applied. One of the dichloromethane solvent molecules is disordered over two adjacent positions about an inversion centre. The highest peak and deepest hole in the difference map are located 1.00 and 0.86 Å, respectively, from atom Ir1.

Data collection: *MSC/AFC Diffractometer Control Software* (Molecular Structure Corporation, 1994); cell refinement: *MSC/AFC Diffractometer Control Software*; data reduction: *MSC/AFC Diffractometer Control Software*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1990); software used to prepare material for publication: *SHELXL97*.

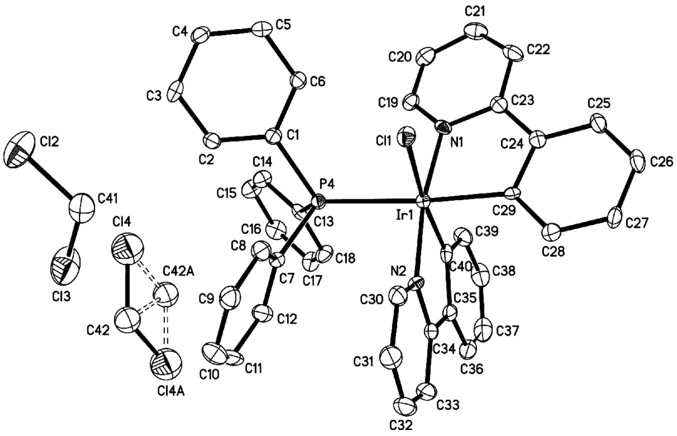


Figure 1
The molecular structure of (I) showing 50% displacement ellipsoids. H atoms have been omitted for clarity. Atoms marked with the suffix A are generated by the symmetry code $(-x, 1 - y, -z)$.

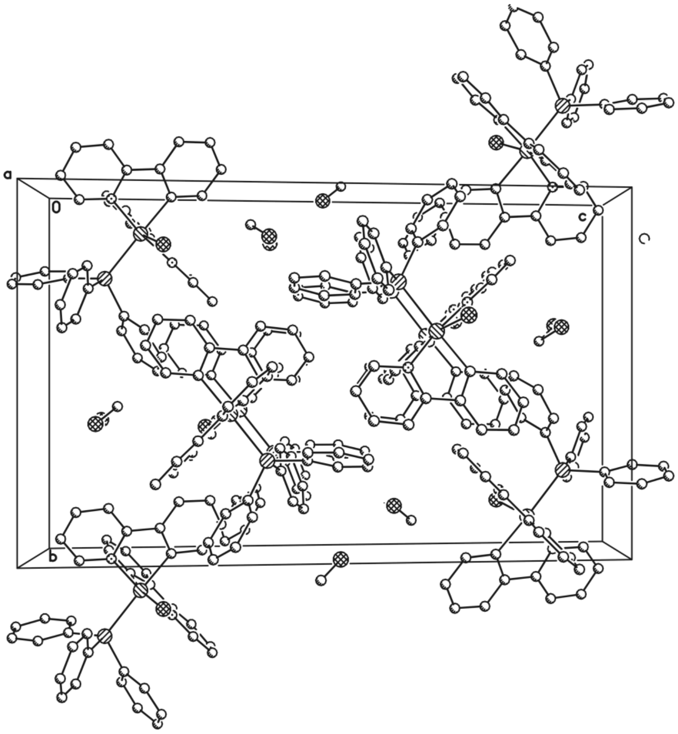


Figure 2
The crystal packing in (I). H atoms have been omitted.

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