The enantiomerically pure iridium title complex, $[\text{Ir}(\text{C}_{12}\text{H}_{19}\text{N}_2\text{O}_2\text{S})(\text{C}_{10}\text{H}_{15})\text{Cl}]\cdot\text{CHCl}_3$, has the Ir atom in the $S$ configuration, with a distorted octahedral geometry.

**Comment**

Recently, we reported an asymmetric transfer hydrogenation reaction in aqueous solution using $\eta^5$-arene ruthenium N-tosyl-trans-1,2-diaminocyclohexane complexes as catalysts (Canivet et al., 2005). In order to extend our studies to iridium complexes, we synthesized the $[\text{Cp}^\ast\text{IrCl}([R,R]-L)]$ complex, (I) $[\text{Cp}^\ast = \text{pentamethylcyclopentadienyl} \text{ and } L\text{H} = (R,R)-N-(p\text{-toluenesulfonyl})-1,2\text{-cyclohexanediamine}]$, which crystallized from chloroform to give a polymorph of the known complex described by Murata et al. (1999). The bond distances and angles are similar to those found in the parent compound $[\text{Cp}^\ast\text{IrCl}([R,R]-L)]$ (Murata et al., 1999), the rhodium analogue $[\text{Cp}^\ast\text{RhCl}([R,R]-L)]$ (Murata et al., 1999) and the nitromethyl derivative $[\text{Cp}^\ast\text{Ir(nitromethyl)}([R,R]-L)]$ (Murata et al., 2002).

The single-crystal X-ray structure analysis of (I) reveals a distorted octahedral geometry for the Ir atom with $\text{Cp}^\ast$, amino, sulfonamido and chloro ligands. Upon formation of complex (I) the iridium metal center becomes chiral. The iridium possesses the $S$ configuration as observed in the ruthenium analogue $[(\eta^5\text{-mesitylene})\text{RuCl}([R,R]-L)]$ [$L\text{H} = (R,R)-N-(p\text{-toluenesulfonyl})-1,2\text{-diphenylthielenediamine}$] (Uematsu et al., 1996) and $[\text{Cp}^\ast\text{IrCl}([R,R]-L)]$.

In contrast with the parent compound which was crystallized from water, (I) was obtained in the presence of chloroform, thus giving rise to a completely different crystal packing. Indeed, two intermolecular hydrogen-bonded systems are observed: an (amino) $\text{N} = \text{H} \cdot \cdot \cdot \text{O} = \text{S}$ (sulfonamido) hydrogen bonding between two symmetry-related molecules and a (chloro) $\text{Ir} = \text{Cl} \cdot \cdot \cdot \text{H} = \text{C}$ (chloroform) hydrogen bonding between complex (I) and the solvent molecule (see Table 1).

**Crystal data**

$[\text{Ir}(\text{C}_{12}\text{H}_{19}\text{N}_2\text{O}_2\text{S})(\text{C}_{10}\text{H}_{15})\text{Cl}]\cdot\text{CHCl}_3$

$M_r = 749.60$

Orthorhombic, $P2_12_12_1$

$a = 9.4012$ (5) Å

$b = 12.8491$ (7) Å

$c = 23.7478$ (17) Å

$V = 2868.7$ (3) Å$^3$

$Z = 4$

$D_\text{r} = 1.736$ Mg m$^{-3}$

Mo $\text{K} \alpha$ radiation

$\mu = 5.12$ mm$^{-1}$

$\theta = 173$ (2) K

Needle, yellow

0.45 $\times$ 0.15 $\times$ 0.08 mm

**Data collection**

Stoe IPDS diffractometer

$\varphi$ scans

Absorption correction: multi-scan

(MULABS in PLATON; Spek, 2003)

$T_{\text{min}} = 0.360$, $T_{\text{max}} = 0.557$

(expected range = 0.428-0.664)

15012 measured reflections

5576 independent reflections

4830 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.044$

$\theta_{\text{max}} = 25.9^\circ$
Refinement

Refinement on $F^2$

$R(F^2 > 2\sigma(F^2)) = 0.028$

$wR(F^2) = 0.059$

$S = 0.94$

3576 reflections

313 parameters

H-atom parameters constrained

$w = 1/\sigma^2(F_o^2) + (0.0306P)^2$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta \sigma)_{\text{max}} = 0.002$

$\Delta \rho_{\text{max}} = 1.53$ e $\text{Å}^{-3}$

$\Delta \rho_{\text{min}} = -1.82$ e $\text{Å}^{-3}$


2413 Friedel pairs

Flack parameter: 0.024 (7)

### Table 1

Hydrogen-bond geometry (Å, °).

<table>
<thead>
<tr>
<th>D—H···A</th>
<th>D—H</th>
<th>H···A</th>
<th>D···A</th>
<th>D—H···A</th>
</tr>
</thead>
<tbody>
<tr>
<td>C24—H24A···Cl1</td>
<td>1.00</td>
<td>2.36</td>
<td>3.357 (8)</td>
<td>178</td>
</tr>
<tr>
<td>N2—H24A···Cl1</td>
<td>0.92</td>
<td>2.60</td>
<td>2.996 (5)</td>
<td>106</td>
</tr>
<tr>
<td>N2—H25B···O2O</td>
<td>0.92</td>
<td>2.26</td>
<td>3.063 (7)</td>
<td>145</td>
</tr>
</tbody>
</table>

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

All H atoms were included in calculated positions (C—H = 0.95 Å for CH$_{\text{arom}}$, 1.00 Å for CH, 0.99 Å for CH$_2$, 0.98 Å for CH$_3$; N—H = 0.92 Å) and treated as riding atoms with the constraint $U_{\text{iso}}(H)$ = 1.2$U_{\text{eq}}$(carrier) applied. The highest residual electron density and deepest hole are both located at less than 1.1 Å from the Ir atom.

Data collection: EXPOSE in IPDS Software (Stoe & Cie, 2000); cell refinement: CELL in IPDS Software; data reduction: INTEGRATE in IPDS Software; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97.

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### References


