

A *p*-cymene-ruthenium(II)–DMSO complex,  
[( $\eta^6$ -C<sub>10</sub>H<sub>14</sub>)RuCl<sub>2</sub>(DMSO)]Manish Chandra,<sup>a</sup> D. Shankar  
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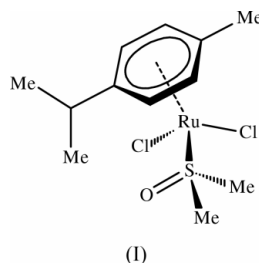
## Key indicators

Single-crystal X-ray study  
T = 293 K  
Mean  $\sigma$ (C–C) = 0.006 Å  
R factor = 0.033  
wR factor = 0.090  
Data-to-parameter ratio = 17.1For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

The crystal structure of the neutral Ru<sup>II</sup> complex [RuCl<sub>2</sub>( $\eta^6$ -C<sub>10</sub>H<sub>14</sub>)(C<sub>2</sub>H<sub>6</sub>OS)] is reported. The overall coordination geometry about the ruthenium centre is best described as a typical 'piano stool'. In the *p*-cymene ligand, the six C atoms of the arene ring are in a planar configuration, as expected.

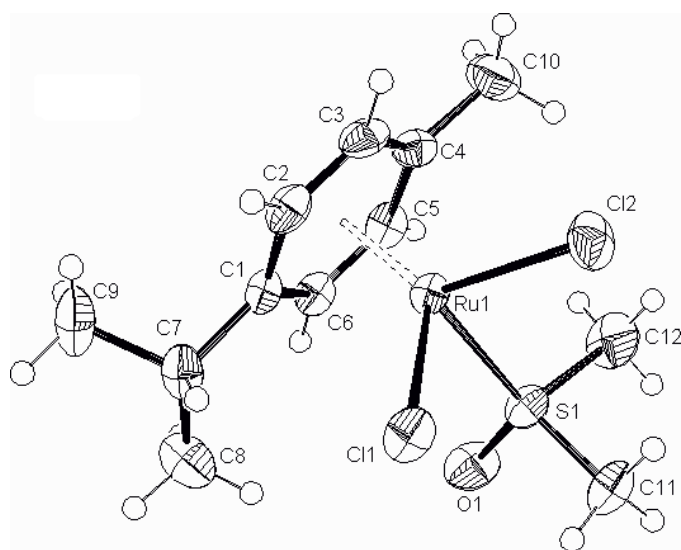
## Comment

The homochiral sulfoxides have received considerable attention recently owing to their prominent role as intermediates in enantioselective synthesis and their potential use as precursors (Schenk *et al.*, 1997; Otto *et al.*, 2001). Because of our continuing interest in the area of arene ruthenium chemistry (Singh *et al.*, 2000), we reacted [( $\eta^6$ -C<sub>10</sub>H<sub>14</sub>)RuCl<sub>2</sub>]<sub>2</sub> with 4-cyanophenyl imidazole, which contained dimethylsulfoxide as solvate. Surprisingly, we isolated the title complex, [( $\eta^6$ -C<sub>10</sub>H<sub>14</sub>)RuCl<sub>2</sub>(DMSO)], (I), instead of the expected arene-ruthenium–organonitrile complex.



The pertinent bond lengths and bond angles may be compared with the closely related 1,4,9,10-tetrahydroanthracene ruthenium complex [( $\eta^6$ -C<sub>14</sub>H<sub>14</sub>)RuCl<sub>2</sub>(DMSO)] (Beasley *et al.*, 1993). The title compound adopts a typical piano-stool geometry (a description commonly used for half-sandwich compounds) with a pseudo-tetrahedral arrangement of the *p*-cymene, the two chloride ligands, and the S atom of the coordinated DMSO ligand around the ruthenium metal centre. This is a similar arrangement to that of [( $\eta^6$ -C<sub>10</sub>H<sub>14</sub>)RuCl<sub>2</sub>(MePPh<sub>2</sub>)], [( $\eta^6$ -C<sub>10</sub>H<sub>14</sub>)RuCl<sub>2</sub>(pz)<sub>2</sub>]PF<sub>6</sub> and the  $\eta^6$ -arene DMSO complex [( $\eta^6$ -C<sub>14</sub>H<sub>14</sub>)RuCl<sub>2</sub>(DMSO)] (Bennett *et al.*, 1972; Tocher *et al.*, 1983; Beasley *et al.*, 1993). The six-membered ring of the *p*-cymene is planar, with a maximum deviation of 0.013 (3) Å (C4) and an overall r.m.s. deviation of 0.008 Å. The C–C bond lengths within the *p*-cymene ring are similar, apart from a shortening of the C2–C3 bond. The Ru–C distances are almost equal, with an average of 2.199 (11) Å. The distance between the centroid of the *p*-cymene ring and ruthenium is 1.683 (3) Å, which is very close to that reported in other Ru<sup>II</sup> arene complexes (Watkins

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**Figure 1**  
The structure of  $[(\eta^6\text{-C}_{10}\text{H}_{14})\text{RuCl}_2(\text{DMSO})]$  showing 50% probability displacement ellipsoids.

& Fronczek, 1982; McCormick *et al.*, 1993; Gupta *et al.*, 1998). The Ru—Cl1 and Ru—Cl2 bond lengths are similar to those in other Ru<sup>II</sup> complexes (Bruce *et al.*, 1981). The DMSO ligand is bonded to ruthenium *via* the S atom, resulting in a roughly tetrahedral arrangement around sulfur. The Ru—S distance is comparable to those observed in the  $\eta^6$ -arene dimethyl sulfoxide complex  $[(\eta^6\text{-C}_{14}\text{H}_{14})\text{RuCl}_2(\text{DMSO})]$  (Beasley *et al.*, 1993) and the Ru<sup>II</sup> complex  $[\text{RuCl}_2(\text{DMSO})_4]$  (Mercer & Trotter, 1975).

## Experimental

The complex  $[(\eta^6\text{-C}_{10}\text{H}_{14})\text{RuCl}_2(\text{DMSO})]$  was prepared in a 68% yield by reaction of  $\{[(\eta^6\text{-C}_{10}\text{H}_{14})\text{RuCl}_2]_2\}$  (0.612 g, 1 mmol) in dichloromethane (25 ml) with 4-cyanophenyl imidazole (0.338 g, 2 mmol) which was previously isolated from dimethyl sulfoxide and therefore contained DMSO as solvate. Orange–red crystals suitable for single-crystal analysis were obtained by slow diffusion of petroleum ether (b.p. 333–353 K) into a solution of the complex in dichloromethane.

### Crystal data

|  |  |
|--|--|
| $[\text{RuCl}_2(\text{C}_{10}\text{H}_{14})(\text{C}_2\text{H}_6\text{OS})]$ | $Z = 2$                                |
| $M_r = 384.31$   | $D_x = 1.692 \text{ Mg m}^{-3}$        |
| Triclinic, $P\bar{1}$  | Mo $K\alpha$ radiation                 |
| $a = 7.8522 (16) \text{ \AA}$  | Cell parameters from 25 reflections    |
| $b = 9.4124 (9) \text{ \AA}$   | $\theta = 5.2\text{--}12.1^\circ$      |
| $c = 10.9151 (17) \text{ \AA}$   | $\mu = 1.51 \text{ mm}^{-1}$           |
| $\alpha = 106.850 (11)^\circ$  | $T = 293 (2) \text{ K}$                |
| $\beta = 94.395 (15)^\circ$  | Needle, brown                          |
| $\gamma = 99.697 (13)^\circ$   | $0.4 \times 0.1 \times 0.1 \text{ mm}$ |
| $V = 754.3 (2) \text{ \AA}^3$  |  |

### Data collection

|   |  |
|---|--|
| Enraf–Nonius CAD-4 diffractometer                               | 2373 reflections with $I > 2\sigma(I)$       |
| $\omega/2\theta$ scans  | $\theta_{\text{max}} = 25.0^\circ$           |
| Absorption correction: $\psi$ scan (North <i>et al.</i> , 1968) | $h = -9 \rightarrow 9$                       |
| $T_{\text{min}} = 0.836$ , $T_{\text{max}} = 0.860$             | $k = 0 \rightarrow 11$                       |
| 2632 measured reflections                                       | $l = -12 \rightarrow 12$                     |
| 2632 independent reflections                                    | 3 standard reflections every 100 reflections |
|   | intensity decay: none                        |

### Refinement

|                                 |  |
|---------------------------------|--|
| Refinement on $F^2$             | H-atom parameters constrained                        |
| $R[F^2 > 2\sigma(F^2)] = 0.033$ | $w = 1/[\sigma^2(F_o^2) + (0.067P)^2]$               |
| $wR(F^2) = 0.090$               | where $P = (F_o^2 + 2F_c^2)/3$                       |
| $S = 1.07$                      | $(\Delta/\sigma)_{\text{max}} = 0.001$               |
| 2632 reflections                | $\Delta\rho_{\text{max}} = 1.26 \text{ e \AA}^{-3}$  |
| 154 parameters                  | $\Delta\rho_{\text{min}} = -0.83 \text{ e \AA}^{-3}$ |

**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

|             |             |            |             |
|-------------|-------------|------------|-------------|
| Ru1—Cl1     | 2.4111 (10) | Ru1—C4     | 2.205 (4)   |
| Ru1—Cl2     | 2.4045 (10) | Ru1—C5     | 2.192 (3)   |
| Ru1—S1      | 2.3400 (10) | Ru1—C6     | 2.181 (3)   |
| Ru1—C1      | 2.201 (3)   | S1—O1      | 1.477 (3)   |
| Ru1—C2      | 2.207 (4)   | S1—C11     | 1.774 (4)   |
| Ru1—C3      | 2.209 (3)   | S1—C12     | 1.784 (4)   |
| Cl1—Ru1—Cl2 | 88.05 (4)   | C12—S1—Ru1 | 109.49 (16) |
| S1—Ru1—Cl1  | 86.28 (4)   | O1—S1—C11  | 108.2 (2)   |
| S1—Ru1—Cl2  | 86.74 (4)   | O1—S1—C12  | 107.5 (2)   |
| O1—S1—Ru1   | 115.71 (13) | C11—S1—C12 | 99.5 (2)    |
| C11—S1—Ru1  | 115.07 (15) |            |             |

The highest residual peak lies 0.919  $\text{\AA}$  from Ru1. All H atoms were placed in calculated positions and refined with a riding model.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *maXus* (Mackay *et al.*, 1998); 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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