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## Key indicators

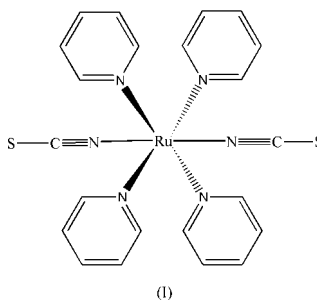
Single-crystal X-ray study  
 $T = 293\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.008\text{ \AA}$   
 $R$  factor = 0.047  
 $wR$  factor = 0.117  
Data-to-parameter ratio = 16.3For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*trans*-Bis(isothiocyanato)tetrapyridine-  
ruthenium(II) dichloromethane disolvate

The title compound, *trans*-[Ru(NCS)<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>4</sub>] $\cdot$ 2CH<sub>2</sub>Cl<sub>2</sub>, was prepared by the reaction between *trans*-dichlorotetrapyridine-ruthenium(II) and excess KSCN in refluxing aqueous pyridine. The Ru atom is in a pseudo-octahedral environment, with two N-donors from two monodentate NCS groups and four N-donors from the pyridine ligands. The complex molecule lies on a crystallographic twofold rotation axis, passing through Ru and the two pyridine ligands

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## Comment

The crystal structure of the title compound, (I), consists of discrete *trans*-[Ru(NCS)<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>4</sub>] molecules and dichloromethane solvent molecules. The Ru atom is coordinated octahedrally by four N atoms from the pyridine ligands and by two N atoms from the monodentate NCS groups in an octahedral arrangement. The Ru–N(C<sub>5</sub>H<sub>5</sub>N) lengths are in the range 2.072 (5)–2.096 (5) Å, close to those in the previously reported compounds *trans*-[Ru(CN)<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>4</sub>] $\cdot$ 2MeCN (Coe *et al.*, 1995*a*) and *trans*-[RuCl(C<sub>5</sub>H<sub>5</sub>N)<sub>4</sub>(PhCN)]PF<sub>6</sub> (Coe *et al.*, 1995*b*). The NCS groups are essentially linear. The N4–C1 [1.159 (5) Å] and C1–S1 [1.632 (4) Å] lengths indicate triple- and single-bond character, respectively, and are similar to those in the reported complexes [Ni(NCS)<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>4</sub>] (Valach *et al.*, 1984) and [Ni(en)<sub>2</sub>(NCS)<sub>2</sub>] $\cdot$ C<sub>6</sub>H<sub>6</sub> (Squattrito *et al.*, 1996). The C–C [1.339 (9)–1.389 (7) Å] and C–N [1.323 (6)–1.346 (5) Å] lengths are in the normal ranges for pyridine ligands (Evans *et al.*, 1973; Coe *et al.*, 1995*a,b*). The mean bond angles in the pyridine ligands [C–N–C = 116.2 (7)°, N–C–C = 123.4 (8)°, and C–C–C = 118.4 (4) and 119.6 (4)°] are similar to those observed in [Ni(NCS)<sub>2</sub>(py)<sub>4</sub>] [C–N–C = 116.8 (5)°, N–C–C = 122.8 (5)°, and C–C–C = 117.1 (6) and 120.2 (6)°; Valach *et al.*, 1984].



## Experimental

The title compound was synthesized by the reaction of a pyridine solution of *trans*-[RuCl<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>4</sub>] (Evans *et al.*, 1973) with an excess of an aqueous solution of KSCN. After refluxing for 1 h, the solution was put aside at room temperature to give a yellow precipitate. The

solid was then filtered off, washed with methanol and ether, and dried in air. Well-shaped crystals were grown by slow diffusion of hexane into a dichloromethane solution at room temperature.

#### Crystal data

[Ru(NCS)<sub>2</sub>(C<sub>5</sub>H<sub>5</sub>N)<sub>4</sub>]<sub>2</sub>·2CH<sub>2</sub>Cl<sub>2</sub>  
*M<sub>r</sub>* = 703.48  
 Monoclinic, *C*2/*c*  
*a* = 12.9410 (8) Å  
*b* = 16.1308 (11) Å  
*c* = 15.4715 (11) Å  
 $\beta$  = 100.988 (2)°  
*V* = 3170.4 (4) Å<sup>3</sup>  
*Z* = 4

*D<sub>x</sub>* = 1.474 Mg m<sup>-3</sup>  
 Mo *K*α radiation  
 Cell parameters from 3186 reflections  
 $\theta$  = 2.0–25.0°  
 $\mu$  = 0.99 mm<sup>-1</sup>  
*T* = 293 (2) K  
 Prism, yellow  
 0.40 × 0.35 × 0.28 mm

#### Data collection

Siemens SMART CCD diffractometer  
 $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
*T<sub>min</sub>* = 0.681, *T<sub>max</sub>* = 0.759  
 4923 measured reflections

2765 independent reflections  
 2352 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.028  
 $\theta_{\max}$  = 25.0°  
*h* = −14 → 15  
*k* = −19 → 10  
*l* = −13 → 18

#### Refinement

Refinement on *F*<sup>2</sup>  
*R*[*F*<sup>2</sup> > 2σ(*F*<sup>2</sup>)] = 0.047  
*wR*(*F*<sup>2</sup>) = 0.117  
*S* = 1.15  
 2765 reflections  
 170 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0355P)^2 + 11.5869P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.51 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.86 \text{ e \AA}^{-3}$

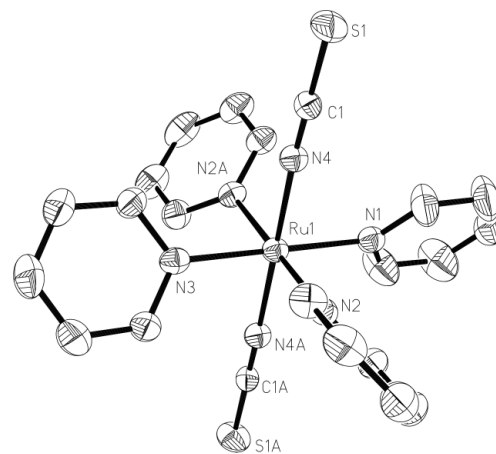
**Table 1**

Selected geometric parameters (Å, °).

Ru1–N4	2.025 (3)	Ru1–N1	2.096 (5)
Ru1–N3	2.072 (5)	S1–C1	1.632 (4)
Ru1–N2	2.082 (3)	N4–C1	1.159 (5)
N4 <sup>i</sup> –Ru1–N4	179.8 (2)	N2 <sup>i</sup> –Ru1–N2	179.7 (2)
N4–Ru1–N3	89.88 (11)	N4–Ru1–N1	90.12 (11)
N4 <sup>i</sup> –Ru1–N2 <sup>i</sup>	88.84 (13)	N2–Ru1–N1	89.84 (11)
N4–Ru1–N2 <sup>i</sup>	91.16 (13)	C1–N4–Ru1	175.6 (3)
N4–Ru1–N2	88.84 (13)	N4–C1–S1	179.9 (5)
N3–Ru1–N2	90.16 (11)		

Symmetry code: (i) 1 − *x*, *y*,  $\frac{3}{2}$  − *z*.

The positions of the H atoms were generated geometrically (C–H bond fixed at 0.96 Å), assigned isotropic displacement parameters, and allowed to ride on their respective parent C atoms.



**Figure 1**

A view of the title complex with the atomic numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) 1 − *x*, *y*,  $\frac{3}{2}$  − *z*.]

Data collection: SMART (Bruker, 1997); cell refinement: SMART; data reduction: SHELXTL (Bruker, 1999); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL; software used to prepare material for publication: SHELXTL.

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