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## Key indicators

Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.007\text{ \AA}$   
 $R$  factor = 0.070  
 $wR$  factor = 0.145  
Data-to-parameter ratio = 14.5For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.*trans*-Bis[(2*E*)-3-(*N,N*-dimethylamino)-1-(2-pyridyl)-  
prop-2-en-1-one]diisothiocyanatonickel(II)

In the title complex,  $[\text{Ni}(\text{NCS})_2(\text{C}_{10}\text{H}_{12}\text{N}_2\text{O})_2]$ , the Ni atom is *trans*-coordinated by two pairs of N and O atoms from two bidentate chelating (2*E*)-3-(*N,N*-dimethylamino)-1-(2-pyridyl)prop-2-en-1-one ligands, and by two N atoms from two isothiocyanate ligands, in a distorted octahedral geometry. The complex is located on an inversion center.

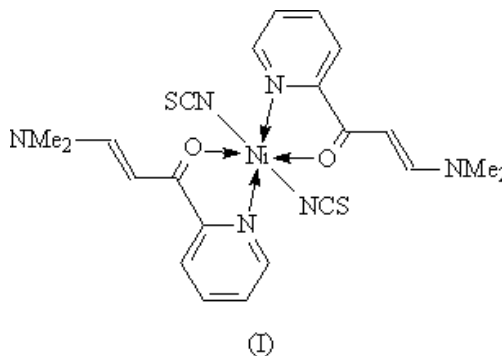
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## Comment

2-Pyridyl ketones are potentially bidentate ligands which may show interesting coordination properties towards metal ions. Some structures have been studied by X-ray diffraction, in which the ligands adopt either a mono- (Kovala-Demertzi *et al.*, 1992; Yang *et al.*, 2000) or bidentate chelating (Sommerer *et al.*, 1998; Goher *et al.*, 1993) coordination mode, depending on the central ions and anions. We report here a nickel complex, *trans*-bis[(2*E*)-3-(*N,N*-dimethylamino)-1-(2-pyridyl)prop-2-en-1-one]diisothiocyanatonickel(II), (I), in which the propenone ligand adopts a bidentate coordination mode.



Complex (I) is located on an inversion center, as shown in Fig. 1. The Ni atom is *trans*-coordinated by two pairs of N and O atoms from two bidentate chelating (2*E*)-3-(*N,N*-dimethylamino)-1-(2-pyridyl)prop-2-en-1-one (*L*) ligands, and by two N atoms from two isothiocyanate ligands, in a distorted octahedral geometry. The five-membered chelate ring formed by the Ni atom and the bidentate ligand *L* is almost planar, the largest deviation being 0.037 (3) Å for atom O1. Atoms C6, C7, C8, N2, C9 and C10 form a plane, the largest deviation being 0.040 (4) Å for C7; this plane is twisted by 12.6 (3)° with respect to the chelate ring. The terminal isothiocyanate group is nearly linear, with an N—C—S angle of 178.7 (5)°, but it is slightly bent at the N atom, making an Ni—N—C angle of 171.9 (5)°. These values may be compared to other nickel complexes containing isothiocyanate ligands (Clemente-Juan *et al.*, 2000).

## Experimental

The (2*E*)-3-(*N,N*-dimethylamino)-1-(2-pyridyl)prop-2-en-1-one (*L*) ligand was synthesized by a modified literature method (Amoroso *et al.*, 1994). A solution of Ni(NCS)<sub>2</sub> (18 mg, 0.1 mmol) in MeOH (10 ml) was carefully layered on top of a solution of *L* (36 mg, 0.2 mmol) in CHCl<sub>3</sub> (10 ml) in a test-tube. After 10 d at room temperature, orange single crystals of (I) appeared at the boundary (yield: 30%). IR (KBr pellet, cm<sup>-1</sup>): 2874 (*w*), 2093 (*s*), 1632 (*s*), 1596 (*m*), 1575 (*m*), 1519 (*s*), 1469 (*m*), 1418 (*s*), 1296 (*m*), 1278 (*m*), 1258 (*s*), 1156 (*m*), 1114 (*m*), 1051 (*m*), 1025 (*m*), 989 (*w*), 905 (*m*), 760 (*m*), 694 (*m*), 648 (*w*), 590 (*m*), 472 (*w*).

### Crystal data

[Ni(NCS) <sub>2</sub> (C <sub>10</sub> H <sub>12</sub> N <sub>2</sub> O) <sub>2</sub> ]	$D_x = 1.443 \text{ Mg m}^{-3}$
$M_r = 527.30$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 912 reflections
$a = 8.086 (4) \text{ \AA}$	$\theta = 3.4\text{--}22.7^\circ$
$b = 10.635 (5) \text{ \AA}$	$\mu = 1.00 \text{ mm}^{-1}$
$c = 14.519 (7) \text{ \AA}$	$T = 298 (2) \text{ K}$
$\beta = 103.614 (8)^\circ$	Block, orange
$V = 1213.5 (10) \text{ \AA}^3$	$0.16 \times 0.07 \times 0.06 \text{ mm}$
$Z = 2$	

### Data collection

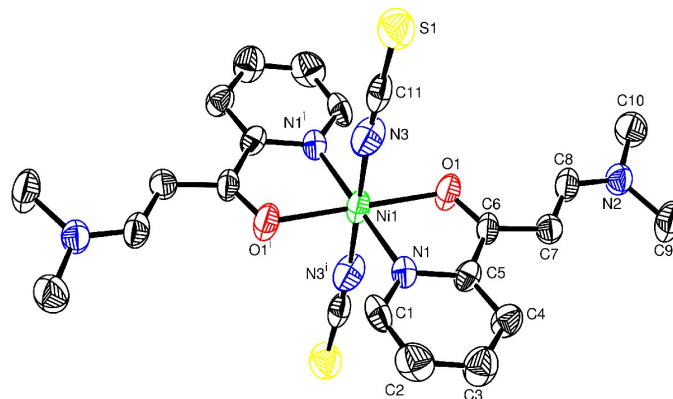
Bruker SMART CCD area-detector diffractometer	2217 independent reflections
$\varphi$ and $\omega$ scans	1325 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$R_{\text{int}} = 0.090$
$T_{\text{min}} = 0.856$ , $T_{\text{max}} = 0.942$	$\theta_{\text{max}} = 25.5^\circ$
6213 measured reflections	$h = -7 \rightarrow 9$
	$k = -12 \rightarrow 12$
	$l = -17 \rightarrow 17$

### Refinement

Refinement on $F^2$	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.070$	$w = 1/[\sigma^2(F_o^2) + (0.0482P)^2]$
$wR(F^2) = 0.145$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.98$	$(\Delta/\sigma)_{\text{max}} = 0.041$
2217 reflections	$\Delta\rho_{\text{max}} = 0.40 \text{ e \AA}^{-3}$
153 parameters	$\Delta\rho_{\text{min}} = -0.39 \text{ e \AA}^{-3}$

H atoms were placed in calculated positions [ $C-H = 0.93$  and  $0.96 \text{ \AA}$ , and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ ] and were included in the refinement in the riding-model approximation.

Data collection: SMART (Bruker, 1998); cell refinement: SMART; data reduction: SAINT (Bruker, 1998) and SHELXTL (Bruker,



**Figure 1**  
View of the title compound, shown with 50% probability ellipsoids [symmetry code: (i)  $-x, -y, -z$ ].

1998); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEPIII (Burnett & Johnson, 1996) and ORTEP-3 for Windows (Farrugia, 1997); software used to prepare material for publication: SHELXTL.

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