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Bis(*N*-phenylpyrazole-1-carboximidothioato-κ^2N^2,S)-nickel(II)

Moayad Hossaini Sadr,[a] Jahanbin Sardroodi,[a] Zohre Shagagi[a] and Seik Weng Ng[b]*

[a]Department of Chemistry, Azarbaijan University of Tarbiat Moallem, Tabriz, Iran, and [b]Department of Chemistry, University of Malaya, 50603 Kuala Lumpur, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.006 Å
R factor = 0.065
wR factor = 0.173
Data-to-parameter ratio = 16.1

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

The Ni atom in the title compound, $[Ni(C_{10}H_8N_3S)_2]$, is *N*,*S*-chelated by two $C_{10}H_8N_3S$ anions in a square-planar geometry. The Ni atom lies on a special position of $\overline{1}$ site symmetry.

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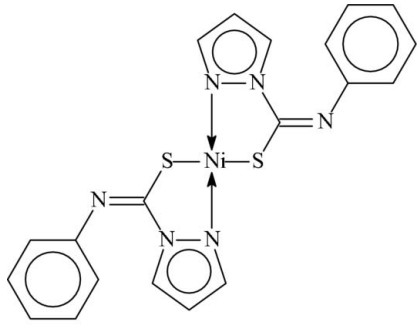
Comment

The crystal structure of a Cu^{II} complex, bis(*N*-phenylpyrazole-1-carboximidothioato)copper(II), has been reported recently by us (Hossain Sadr *et al.*, 2005). The title Ni^{II} complex, (I), is isostructural with the Cu^{II} complex.



(I)

The molecular structure of (I) is shown in Fig. 1. The Ni^{II} atom exists in a square-planar N_2S_2Ni geometry with normal coordination bond distances and angles (Table 1). The metal atom lies on a centre of inversion.

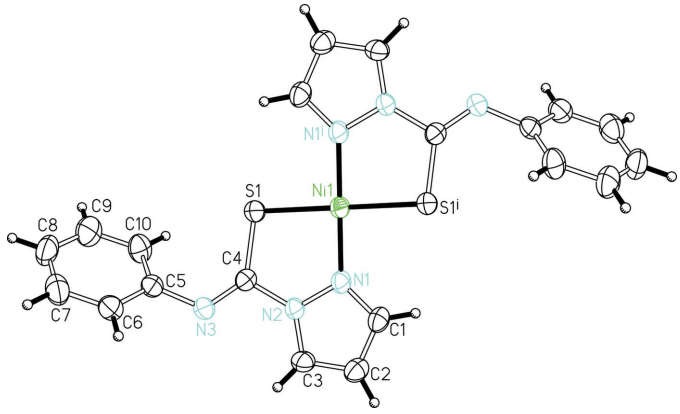


Figure 1
A plot of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radii. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

Experimental

Nickel(II) chloride (0.13 g, 1 mmol) and sodium *N*-phenyl-2-pyrazolyl-1-carboximidothioate (0.50 g 2.2 mmol) were stirred in methanol (50 ml) for several hours to yield a precipitate; this was collected and recrystallized from tetrahydrofuran (30 ml) to yield needle crystals of (I).

Crystal data

$[Ni(C_{10}H_8N_3S)_2]$
$M_r = 463.22$
Monoclinic, $P2_1/c$
$a = 5.9847\ (5)$ Å
$b = 21.365\ (2)$ Å
$c = 7.8700\ (6)$ Å
$\beta = 103.605\ (1)^\circ$
$V = 978.05\ (14)$ Å^3
$Z = 2$
$D_x = 1.573$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2454 reflections
$\theta = 2.8$–27.0°
$\mu = 1.23$ mm^{-1}
$T = 295\ (2)$ K
Needle, red–brown
$0.43 \times 0.16 \times 0.07$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.453$, $T_{max} = 0.919$
6319 measured reflections
2147 independent reflections
1655 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 27.2^\circ$
$h = -7 \rightarrow 7$
$k = -25 \rightarrow 27$
$l = -9 \rightarrow 10$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.065$
$wR(F^2) = 0.173$
$S = 1.10$
2147 reflections
133 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1055P)^2 + 0.0972P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.40$ e Å^{-3}
$\Delta\rho_{min} = -0.83$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Ni1—N1	1.869 (3)	Ni1—S1	2.194 (1)
N1—Ni1—S1	87.45 (9)		

H atoms were positioned geometrically, with C—H = 0.93 Å, and were included in the refinement in the riding-model approximation, with $U_{iso}(H) = 1.2U_{eq}(C)$. The final difference Fourier map has a large peak at about 1 Å from atom Ni1.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; method used to solve structure: atomic coordinates taken from the isostructural Cu analogue (Hossain Sadr *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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