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Bis(quinoxaline-2,3-dithiolato-*S*,*S*′)nickel(II)

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Key indicators

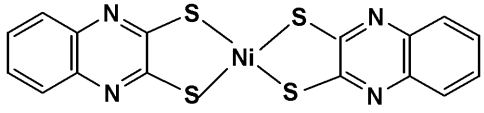
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.009 Å
R factor = 0.059
wR factor = 0.163
Data-to-parameter ratio = 12.0

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

The title complex, $[Ni(C_8H_4N_2S_2)_2]$, is a mononuclear nickel(II) complex in which the coordination about the Ni atom to the four S atoms of the two quinoxaline-2,3-dithiolate (qt) ligands is slightly distorted square planar. The molecule has a crystallographic inversion centre.

Comment

Thiolates are a subject of great interest in the chemistry of transition metal complexes (Krebs & Henkel, 1991). In an attempt to synthesize new complexes with novel electric and magnetic properties (Sheng *et al.*, 1998), we reacted $Ni(CH_3COO)_2$ with quinoxaline-2,3-dithiol and the unpredicted title compound $[Ni(qt)_2]$, (I), was isolated.



(I)

As shown in Fig. 1, (I) is a mononuclear nickel(II) complex consisting of two quinoxaline-2,3-dithiolate (qt) ligands and one Ni^{II} atom. The coordination about the Ni atom is slightly distorted square planar. The bond distances Ni—S are 2.1664 (15) and 2.1850 (15) Å. The angles S1—Ni—S2 and S1—Ni—S2*A* are 91.67 (5) and 88.33 (5)°, respectively.

Experimental

The title compound, (I), was obtained from the reaction of $Ni(ac)_2$ (1 mmol) and qt (2 mmol) in CH_3OH (15 ml). $Ni(Ac)_2$ (1 mmol) and qt (2 mmol) were sealed in a steel reactor with 15 ml of CH_3OH. The reaction mixture was heated to 363 K and maintained at this temperature for 72 h. After the reaction the solution was cooled to room temperature and a large amount of dark-brown and sheet-like crystals was obtained.

Crystal data

$[Ni(C_8H_4N_2S_2)_2]$
M_r = 443.23
Monoclinic, $P2_1/c$
a = 6.6528 (2) Å
b = 5.7251 (2) Å
c = 20.9637 (8) Å
β = 90.205 (2)°
V = 798.46 (5) Å^3
Z = 4
D_x = 1.843 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1378 reflections
θ = 1.9–25.0°
μ = 1.75 mm^{-1}
T = 293 (2) K
Sheet, black
0.24 × 0.18 × 0.08 mm

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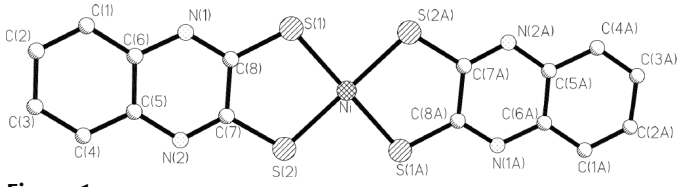

Figure 1
The structure of bis(quinoxaline-2,3-dithiolato-*S*,*S*′)nickel(II).

Data collection

SMART CCD diffractometer
ω scans
Absorption correction: empirical *SHELXTL* (Siemens,1994)
T_{min} = 0.492, T_{max} = 0.794
2114 measured reflections
1378 independent reflections
1022 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 25.0°
$h = -7 \rightarrow 4$
$k = -6 \rightarrow 3$
$l = -22 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.059$
$wR(F^2) = 0.163$
$S = 1.05$
1378 reflections
115 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0965P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.89$ e Å^{-3}
$\Delta\rho_{min} = -0.65$ e Å^{-3}

The positions of all H atoms were generated geometrically (C—H distance fixed at 0.96 Å), assigned isotropic displacement parameters and allowed to ride on their respective parent C atoms in the final cycle of least-squares refinement.

Data collection: *SMART* (Siemens, 1994); cell refinement: *SMART*; data reduction: *SAINT* (Siemens, 1994); program(s) used to solve structure: *SHELX*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELX*97; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*.

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