

catena-Poly[[bis(*O,O'*-dicyclohexyl dithiophosphato- κ^2S,S')nickel(II)]- μ -4,4'-bipyridine- $\kappa^2N:N'$]

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Key indicators

Single-crystal X-ray study
 $T = 120$ K
 Mean $\sigma(C-C) = 0.011$ Å
 Disorder in main residue
 R factor = 0.060
 wR factor = 0.193
 Data-to-parameter ratio = 14.4

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

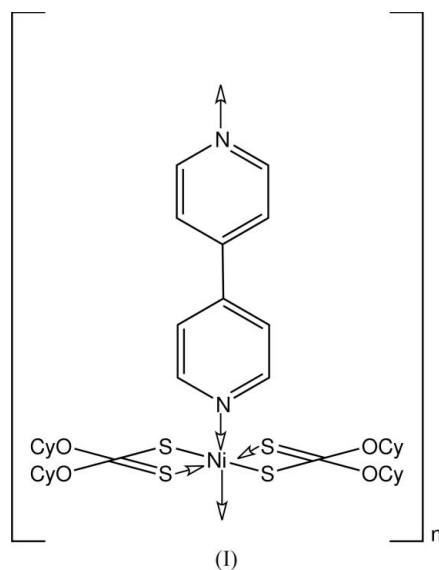
The Ni atom in the linear polymeric title complex, $[Ni\{S_2P(OC_6H_{11})_2\}_2(NC_5H_4C_5H_4N)]_n$ or $[Ni(C_{12}H_{22}O_2PS_2)_2(C_{10}H_8N_2)]_n$, is octahedrally coordinated within a *trans*- N_2S_4 donor set. The Ni atom and the N atoms of the 4,4'-bipyridine ligand are located on a twofold axis.

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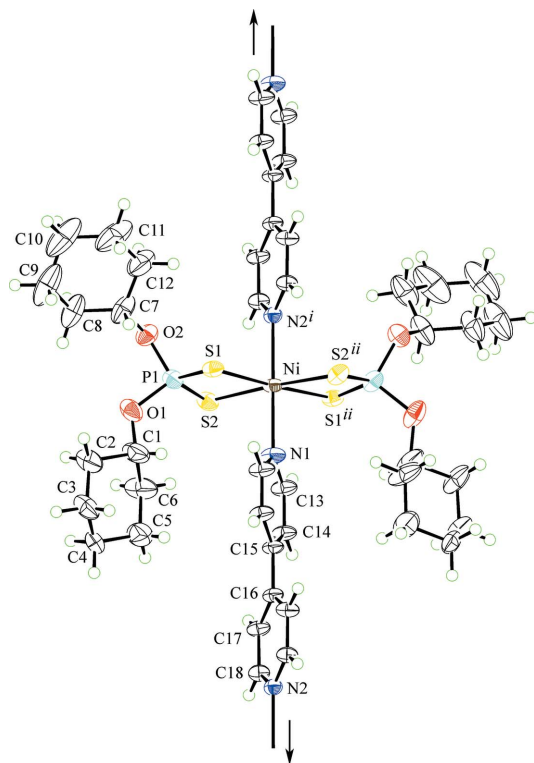
Comment

The title compound, (I), was investigated as an extension of our interest in generating coordination polymers of metal dithiophosphates (*e.g.* Lai *et al.* 2004; Lai & Tiekink, 2004; Chen *et al.*, 2006). The asymmetric unit in (I) comprises one Ni atom (site symmetry 2), half a 4,4'-bipyridine ligand, and one dithiophosphate ligand. The structure has crystallographic twofold symmetry in that the $N \cdots N$ axis of the 4,4'-bipyridine ligand as well as the Ni atom lie on a twofold axis. The dihedral angle between the mean planes of the N1 and N2 rings of the 4,4'-bipyridine molecule is 37.9 (2)°.

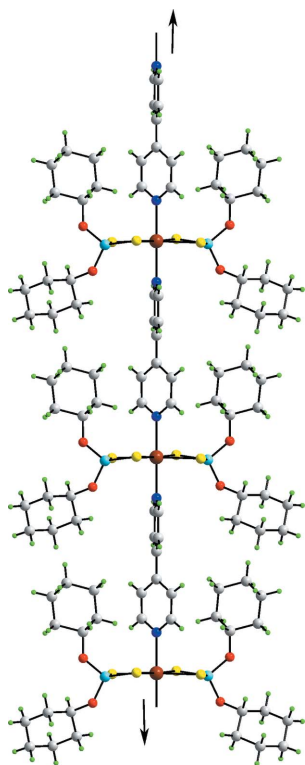


The coordination polyhedron for the Ni atom is an octahedron defined by a *trans*- N_2S_4 donor set, with the N atoms provided by bridging 4,4'-bipyridine ligands and S atoms from two symmetrically chelating dithiophosphate ligands (Fig. 1 and Table 1).

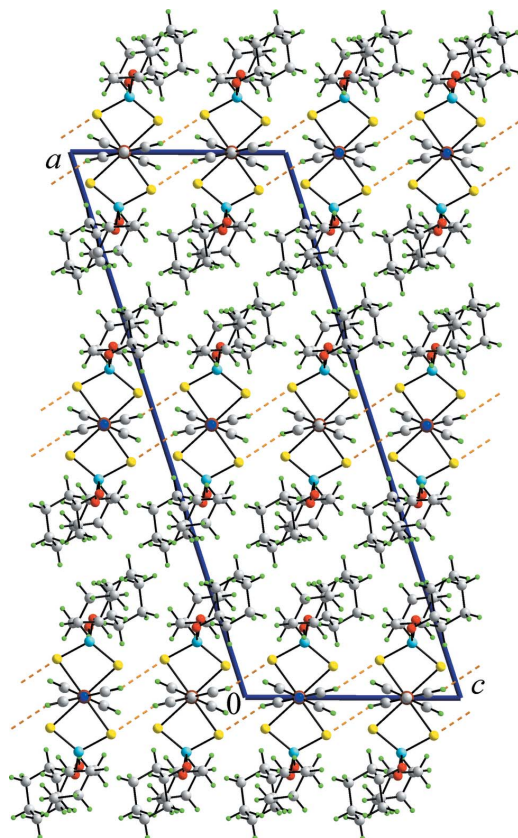
The polymer topology in (I) is linear (Fig. 2). While it is well known that $Ni[S_2P(OR)_2]_2$ complexes can form six-coordinate adducts with bipyridine-type bases (*e.g.* Berdugo & Tiekink, 2006; Berdugo *et al.*, 2006), the structure of (I) represents the first example of a polymer being formed in such species. In the crystal structure, polymers are aligned along the *b* axis and

**Figure 1**

Asymmetric unit of (I) expanded to show the polymeric connectivity. Only the major component of the disorder is shown. Displacement ellipsoids are shown at the 50% probability level (arbitrary spheres for the H atoms). [Symmetry codes: (i) $x, y - 1, z$; (ii) $-x, y, -z + \frac{1}{2}$.]

**Figure 2**

View of the linear polymer in (I). Colour code: Zn (brown), S (yellow), P (pale blue), O (red), N (dark blue), C (grey) & H (green). Only the major disorder component is shown.

**Figure 3**

View of the unit-cell contents of (I) down the b axis, showing the weak $C-H \cdots S$ connections (dashed lines) between chains. Colour code as for Fig. 2. Only the major disorder component is shown.

pack in layers stacked along the a axis separated by hydrophobic interactions (Fig. 3). Within layers, the chains are offset so as to allow for the formation of weak $C-H \cdots S$ interactions between a phenyl H atom of the 4,4'-bipyridine bridge and the acceptor S2 atom in an adjacent chain (Table 2).

Experimental

The title compound was prepared by refluxing the parent nickel(II) dithiophosphate with 4,4'-bipyridine, following a literature procedure (Lai *et al.*, 2004). Light-green crystals were isolated by the slow evaporation of an acetonitrile/ $CHCl_3$ (1:3) solution of the complex.

Crystal data

[Ni(C₁₂H₂₂O₂PS₂)₂(C₁₀H₈N₂)]
 $M_r = 801.67$
 Monoclinic, $C2/c$
 $a = 30.709$ (2) Å
 $b = 11.4278$ (8) Å
 $c = 11.5210$ (4) Å
 $\beta = 108.009$ (3)°

$V = 3845.1$ (4) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.84$ mm⁻¹
 $T = 120$ (2) K
 $0.20 \times 0.10 \times 0.02$ mm

Data collection

Bruker-Nonius KappaCCD diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
 $T_{min} = 0.747$, $T_{max} = 1$

23861 measured reflections
 3393 independent reflections
 2047 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.138$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.060$	236 parameters
$wR(F^2) = 0.193$	H-atom parameters constrained
$S = 1.10$	$\Delta\rho_{\max} = 0.62 \text{ e } \text{\AA}^{-3}$
3393 reflections	$\Delta\rho_{\min} = -0.84 \text{ e } \text{\AA}^{-3}$

Table 1

Selected bond lengths (Å).

Ni—S1	2.4721 (13)	Ni—N1	2.158 (7)
Ni—S2	2.4865 (16)	Ni—N2 ⁱ	2.160 (6)

Symmetry code: (i) $x, y - 1, z$.

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C14—H14 ⁱⁱ ··S2 ⁱⁱⁱ	0.95	2.86	3.604 (5)	136

Symmetry code: (iii) $-x, -y - 1, -z$.

The relatively high value for R_{int} is ascribed to the poor quality of the crystals and the internal disorder in the structure. The H atoms were geometrically placed ($C-H = 0.95-1.00\text{\AA}$) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl C})$. Disorder was modelled for the O1 cyclohexyl group in that two positions were resolved for the C atoms [occupancy of the major component = 0.755 (11)]. The C atoms of the minor component were refined isotropically.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT*; data reduc-

tion: *DENZO* and *COLLECT*; program(s) used to solve structure: *PATY* in *DIRDIF92* (Beurskens *et al.*, 1992); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

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