Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

Erick Berdugo,[a] Edward R. T. Tiekink,[a]* James L. Wardell[a,b] and Solange M. S. V. Wardell[c]

[a]Department of Chemistry, The University of Texas at San Antonio, One UTSA Circle, San Antonio, Texas 78249-0698, USA, [b]Department of Chemistry, University of Aberdeen, Old Aberdeen AB24 3UE, Scotland, and [c]Complexo Tecnológico de Medicamentos Farmanguinhos, Av. Comandante Guaranys 447, Jacarepaguá, Rio de Janeiro, RJ, Brazil

Correspondence e-mail: edward.tiekink@utsa.edu

Key indicators

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

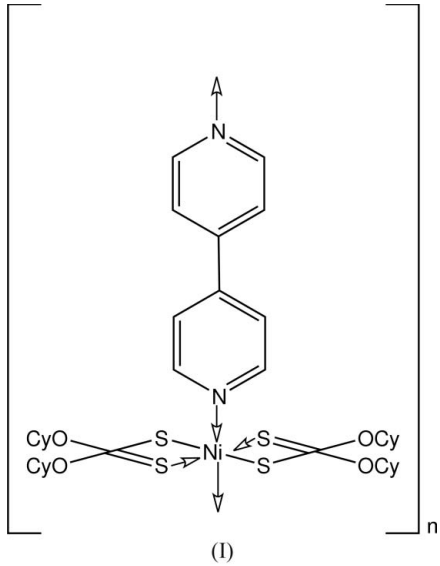
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 7 February 2007
Accepted 8 February 2007

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.

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···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)°.



(I)

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

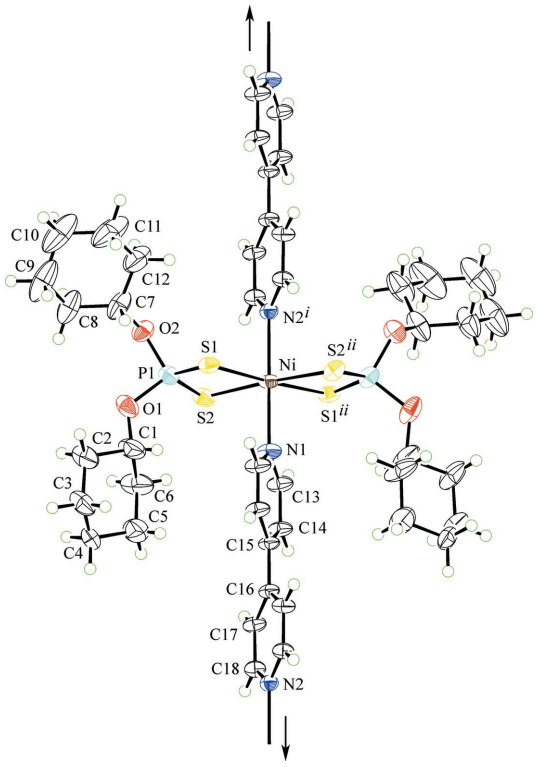


Figure 1
Asymmetric unit of (I) expanded to show the polymeric connectivity. Only the major component of the disorder is shown. Displacement ellipsoids are shown at the 50% probability level (arbitrary spheres for the H atoms). [Symmetry codes: (i) $x, y-1, z$; (ii) $-x, y, -z+\frac{1}{2}$.]

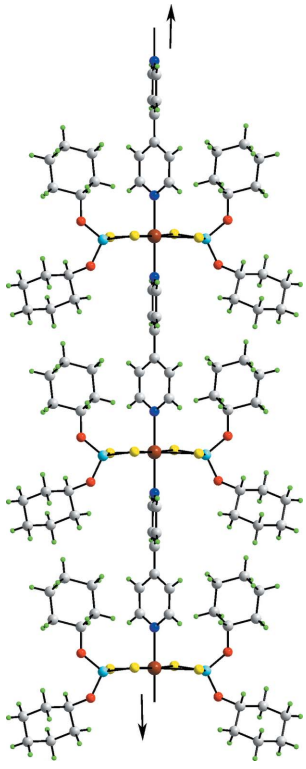


Figure 2
View of the linear polymer in (I). Colour code: Zn (brown), S (yellow), P (pale blue), O (red), N (dark blue), C (grey) & H (green). Only the major disorder component is shown.

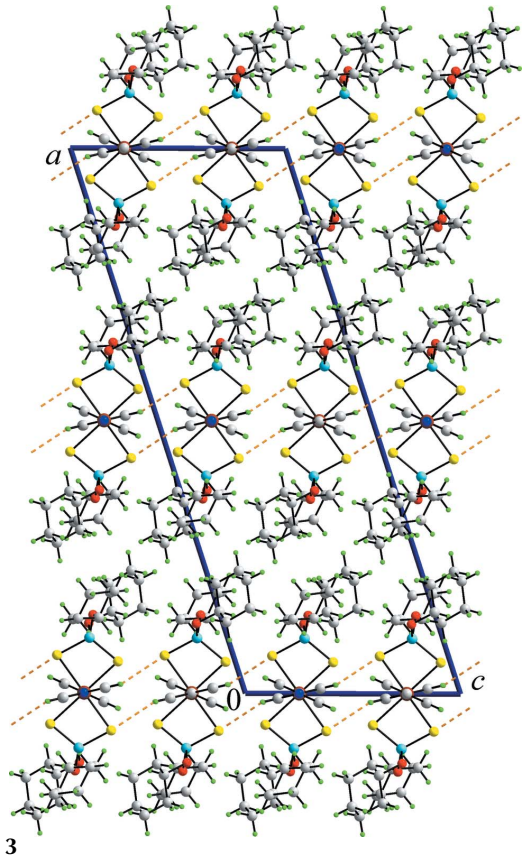


Figure 3
View of the unit-cell contents of (I) down the *b* axis, showing the weak C—H···S connections (dashed lines) between chains. Colour code as for Fig. 2. Only the major disorder component is shown.

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···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 nicke(II)l 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

$[Ni(C_{12}H_{22}O_2PS_2)_2(C_{10}H_8N_2)]$
$M_r = 801.67$
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) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.84$ mm^{-1}
$T = 120$ (2) K
0.20 × 0.10 × 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
$S = 1.10$	$\Delta\rho_{max} = 0.62$ e Å^{-3}
3393 reflections	$\Delta\rho_{min} = -0.84$ e Å^{-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···A	D—H	H···A	D···A	D—H···A
C14—H14···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 = 0.95–1.00Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(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 reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: PATTY 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*.

This work was supported by the departmental research grant AX-0026 from The Robert A. Welch Foundation. Cheminova is thanked for the gift of the dithiophosphate ligand used in this study.

References

Berdugo, E. & Tiekink, E. R. T. (2006). *Acta Cryst.* E**62**, m2218–m2220.
Berdugo, E., Tiekink, E. R. T., Wardell, J. L. & Wardell, S. M. S. V. (2006). *Acta Cryst.* E**62**, m2693–m2694.
Beurskens, P. T., Admiraal, G., Beurskens, G., Bosman, W. P., Garcia-Granda, S., Gould, R. O., Smits, J. M. M. & Smykalla, C. (1992). *The DIRDIF Program System*. Technical Report. Crystallography Laboratory, University of Nijmegen, The Netherlands.
Brandenburg, K. (2006). *DIAMOND*. Release 3.1. Crystal Impact GbR, Bonn, Germany.
Chen, D., Lai, C. S. & Tiekink, E. R. T. (2006). *CrystEngComm*, **8**, 51–58.
Hooft, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Lai, C. S., Liu, S. & Tiekink, E. R. T. (2004). *CrystEngComm*, **6**, 221–226.
Lai, C. S. & Tiekink, E. R. T. (2004). *CrystEngComm*, **6**, 593–605.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. Bruker AXS Inc., Madison, Wisconsin, USA.

supporting information

Acta Cryst. (2007). E**63**, m764–m766 [https://doi.org/10.1107/S1600536807006757]

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

Erick Berdugo, Edward R. T. Tiekink, James L. Wardell and Solange M. S. V. Wardell

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

Crystal data

$[Ni(C_{12}H_{22}O_2PS_2)_2(C_{10}H_8N_2)]$
$M_r = 801.67$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
$a = 30.709\ (2)$ Å
$b = 11.4278\ (8)$ Å
$c = 11.5210\ (4)$ Å
$\beta = 108.009\ (3)°$
$V = 3845.1\ (4)$ Å^3
$Z = 4$
$F(000) = 1696$
$D_x = 1.385$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 4564 reflections
$\theta = 1.0–27.5°$
$\mu = 0.84$ mm^{-1}
$T = 120$ K
Plate, light-green
0.20 × 0.10 × 0.02 mm

Data collection

Bruker–Nonius KappaCCD diffractometer
Radiation source: Bruker–Nonius FR591 rotating-anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)
$T_{min} = 0.747$, $T_{max} = 1$
23861 measured reflections
3393 independent reflections
2047 reflections with $I > 2\sigma(I)$
$R_{int} = 0.138$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.4°$
$h = -36\rightarrow36$
$k = -13\rightarrow13$
$l = -13\rightarrow13$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.060$
$wR(F^2) = 0.193$
$S = 1.10$
3393 reflections
236 parameters
24 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1034P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.62$ e Å^{-3}
$\Delta\rho_{min} = -0.84$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni	0.0000	−0.68498 (8)	0.2500	0.0284 (3)	
S1	0.05769 (5)	−0.69028 (12)	0.45448 (11)	0.0323 (4)	
S2	0.06899 (5)	−0.67863 (14)	0.18054 (12)	0.0369 (4)	
P1	0.10119 (5)	−0.69928 (14)	0.35736 (13)	0.0370 (4)	
O2	0.12774 (14)	−0.8203 (4)	0.3758 (3)	0.0423 (11)	
N1	0.0000	−0.4961 (6)	0.2500	0.0376 (18)	
N2	0.0000	0.1260 (6)	0.2500	0.0279 (15)	
O1	0.14322 (15)	−0.6130 (4)	0.4082 (3)	0.0529 (13)	0.755 (11)
C1	0.1379 (3)	−0.4913 (6)	0.4305 (6)	0.075 (3)	0.755 (11)
H1	0.1113	−0.4743	0.4604	0.090*	0.755 (11)
C2	0.1842 (4)	−0.4576 (8)	0.5216 (8)	0.064 (4)	0.755 (11)
H2A	0.1883	−0.4982	0.6001	0.077*	0.755 (11)
H2B	0.2092	−0.4826	0.4897	0.077*	0.755 (11)
C3	0.1868 (3)	−0.3282 (7)	0.5419 (6)	0.059 (3)	0.755 (11)
H3A	0.2168	−0.3078	0.6011	0.070*	0.755 (11)
H3B	0.1626	−0.3038	0.5770	0.070*	0.755 (11)
C4	0.1808 (3)	−0.2634 (7)	0.4237 (6)	0.048 (3)	0.755 (11)
H4A	0.1812	−0.1780	0.4385	0.058*	0.755 (11)
H4B	0.2064	−0.2825	0.3919	0.058*	0.755 (11)
C5	0.1362 (3)	−0.2974 (7)	0.3314 (8)	0.074 (4)	0.755 (11)
H5A	0.1105	−0.2755	0.3619	0.089*	0.755 (11)
H5B	0.1324	−0.2548	0.2541	0.089*	0.755 (11)
C6	0.1353 (4)	−0.4279 (7)	0.3087 (6)	0.076 (4)	0.755 (11)
H6A	0.1617	−0.4508	0.2813	0.091*	0.755 (11)
H6B	0.1068	−0.4498	0.2442	0.091*	0.755 (11)
O21	0.14322 (15)	−0.6130 (4)	0.4082 (3)	0.0529 (13)	0.245 (11)
C21	0.1379 (3)	−0.4913 (6)	0.4305 (6)	0.075 (3)	0.245 (11)
H21	0.1139	−0.4991	0.4723	0.090*	0.245 (11)
C22	0.1759 (7)	−0.441 (2)	0.5370 (12)	0.09 (2)*	0.245 (11)
H22A	0.1879	−0.5009	0.6005	0.105*	0.245 (11)
H22B	0.1642	−0.3742	0.5739	0.105*	0.245 (11)
C23	0.2131 (4)	−0.400 (2)	0.4863 (18)	0.056 (9)*	0.245 (11)
H23A	0.2379	−0.3618	0.5520	0.068*	0.245 (11)
H23B	0.2264	−0.4678	0.4562	0.068*	0.245 (11)
C24	0.1947 (6)	−0.315 (2)	0.3844 (19)	0.055 (8)*	0.245 (11)

H24A	0.1874	−0.2407	0.4187	0.066*	0.245 (11)
H24B	0.2190	−0.2977	0.3468	0.066*	0.245 (11)
C25	0.1531 (6)	−0.3556 (19)	0.2870 (14)	0.048 (8)*	0.245 (11)
H25A	0.1609	−0.4232	0.2435	0.057*	0.245 (11)
H25B	0.1413	−0.2921	0.2271	0.057*	0.245 (11)
C26	0.1163 (5)	−0.3913 (16)	0.3448 (17)	0.045 (8)*	0.245 (11)
H26A	0.1086	−0.3252	0.3904	0.054*	0.245 (11)
H26B	0.0881	−0.4176	0.2816	0.054*	0.245 (11)
C7	0.1497 (2)	−0.8618 (7)	0.5007 (5)	0.055 (2)	
H7	0.1426	−0.8051	0.5585	0.066*	
C8	0.2010 (3)	−0.8640 (8)	0.5250 (6)	0.072 (2)	
H8A	0.2120	−0.7843	0.5148	0.087*	
H8B	0.2085	−0.9161	0.4652	0.087*	
C9	0.2247 (3)	−0.9069 (11)	0.6524 (7)	0.098 (4)	
H9A	0.2581	−0.9114	0.6654	0.118*	
H9B	0.2196	−0.8505	0.7120	0.118*	
C10	0.2075 (4)	−1.0245 (11)	0.6737 (7)	0.107 (4)	
H10A	0.2225	−1.0484	0.7594	0.128*	
H10B	0.2155	−1.0827	0.6199	0.128*	
C11	0.1562 (4)	−1.0221 (9)	0.6481 (8)	0.106 (4)	
H11A	0.1487	−0.9709	0.7085	0.128*	
H11B	0.1453	−1.1020	0.6576	0.128*	
C12	0.1307 (3)	−0.9768 (8)	0.5171 (7)	0.075 (3)	
H12A	0.1349	−1.0327	0.4557	0.090*	
H12B	0.0976	−0.9696	0.5059	0.090*	
C13	−0.0092 (2)	−0.4345 (5)	0.1460 (5)	0.0394 (16)	
H13	−0.0160	−0.4761	0.0712	0.047*	
C14	−0.0093 (2)	−0.3145 (5)	0.1424 (4)	0.0349 (14)	
H14	−0.0158	−0.2752	0.0662	0.042*	
C15	0.0000	−0.2499 (7)	0.2500	0.0307 (19)	
C16	0.0000	−0.1210 (7)	0.2500	0.0285 (18)	
C17	0.0168 (2)	−0.0568 (5)	0.1702 (4)	0.0327 (14)	
H17	0.0286	−0.0961	0.1137	0.039*	
C18	0.01619 (19)	0.0637 (5)	0.1732 (4)	0.0301 (13)	
H18	0.0279	0.1052	0.1179	0.036*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni	0.0411 (6)	0.0168 (6)	0.0235 (5)	0.000	0.0042 (4)	0.000
S1	0.0454 (9)	0.0238 (8)	0.0238 (7)	−0.0008 (7)	0.0049 (6)	0.0005 (6)
S2	0.0442 (9)	0.0361 (10)	0.0268 (7)	−0.0097 (8)	0.0061 (6)	0.0039 (6)
P1	0.0409 (10)	0.0377 (10)	0.0276 (8)	−0.0082 (8)	0.0037 (6)	0.0050 (7)
O2	0.045 (2)	0.046 (3)	0.035 (2)	0.009 (2)	0.0117 (18)	0.0096 (19)
N1	0.061 (5)	0.024 (4)	0.024 (3)	0.000	0.006 (3)	0.000
N2	0.032 (4)	0.024 (4)	0.025 (3)	0.000	0.004 (3)	0.000
O1	0.049 (3)	0.059 (3)	0.039 (2)	−0.022 (2)	−0.004 (2)	0.013 (2)
C1	0.074 (6)	0.048 (5)	0.073 (5)	−0.028 (4)	−0.021 (4)	0.016 (4)

C2	0.071 (8)	0.063 (8)	0.034 (5)	−0.030 (6)	−0.019 (5)	0.012 (5)
C3	0.061 (6)	0.058 (7)	0.053 (6)	−0.028 (5)	0.012 (5)	−0.007 (5)
C4	0.035 (5)	0.045 (6)	0.060 (6)	−0.015 (4)	0.009 (4)	−0.002 (5)
C5	0.066 (7)	0.058 (8)	0.079 (7)	−0.013 (6)	−0.005 (6)	0.013 (6)
C6	0.109 (10)	0.044 (7)	0.042 (5)	−0.025 (7)	−0.024 (6)	−0.002 (5)
O21	0.049 (3)	0.059 (3)	0.039 (2)	−0.022 (2)	−0.004 (2)	0.013 (2)
C21	0.074 (6)	0.048 (5)	0.073 (5)	−0.028 (4)	−0.021 (4)	0.016 (4)
C7	0.053 (4)	0.083 (6)	0.030 (3)	0.030 (4)	0.017 (3)	0.019 (3)
C8	0.055 (5)	0.103 (7)	0.049 (4)	0.031 (5)	0.000 (3)	0.002 (4)
C9	0.079 (7)	0.156 (11)	0.044 (5)	0.063 (7)	−0.003 (4)	−0.006 (5)
C10	0.117 (9)	0.149 (11)	0.054 (5)	0.083 (8)	0.026 (5)	0.034 (6)
C11	0.127 (9)	0.114 (9)	0.091 (6)	0.066 (7)	0.054 (6)	0.065 (6)
C12	0.071 (6)	0.080 (6)	0.082 (5)	0.031 (5)	0.037 (4)	0.039 (5)
C13	0.066 (4)	0.023 (3)	0.024 (3)	0.000 (3)	0.005 (3)	−0.002 (2)
C14	0.058 (4)	0.021 (3)	0.021 (3)	−0.001 (3)	0.005 (3)	0.002 (2)
C15	0.044 (5)	0.015 (4)	0.028 (4)	0.000	0.004 (4)	0.000
C16	0.041 (5)	0.018 (4)	0.021 (4)	0.000	0.002 (3)	0.000
C17	0.051 (4)	0.021 (3)	0.025 (3)	0.003 (3)	0.011 (3)	−0.001 (2)
C18	0.042 (4)	0.024 (3)	0.026 (3)	0.001 (3)	0.013 (2)	−0.002 (2)

Geometric parameters (Å, º)

Ni—S1	2.4721 (13)	C22—H22B	0.9900
Ni—S2	2.4865 (16)	C23—C24	1.492 (10)
Ni—N1	2.158 (7)	C23—H23A	0.9900
Ni—N2^{i}	2.160 (6)	C23—H23B	0.9900
Ni—S1^{ii}	2.4721 (13)	C24—C25	1.491 (10)
Ni—S2^{ii}	2.4865 (16)	C24—H24A	0.9900
S1—P1	1.993 (2)	C24—H24B	0.9900
S2—P1	1.9844 (19)	C25—C26	1.534 (10)
P1—O2	1.586 (4)	C25—H25A	0.9900
P1—O21	1.585 (4)	C25—H25B	0.9900
P1—O1	1.585 (4)	C26—H26A	0.9900
O2—C7	1.466 (7)	C26—H26B	0.9900
N1—C13	1.342 (6)	C7—C12	1.473 (11)
N1—C13^{ii}	1.342 (6)	C7—C8	1.513 (9)
N2—C18	1.345 (6)	C7—H7	1.0000
N2—C18^{ii}	1.345 (6)	C8—C9	1.505 (9)
N2—Ni^{iii}	2.160 (6)	C8—H8A	0.9900
O1—C1	1.433 (9)	C8—H8B	0.9900
C1—C2	1.533 (7)	C9—C10	1.492 (14)
C1—C6	1.560 (7)	C9—H9A	0.9900
C1—H1	1.0000	C9—H9B	0.9900
C2—C3	1.495 (9)	C10—C11	1.512 (14)
C2—H2A	0.9900	C10—H10A	0.9900
C2—H2B	0.9900	C10—H10B	0.9900
C3—C4	1.511 (7)	C11—C12	1.557 (9)
C3—H3A	0.9900	C11—H11A	0.9900

C3—H3B	0.9900	C11—H11B	0.9900
C4—C5	1.503 (7)	C12—H12A	0.9900
C4—H4A	0.9900	C12—H12B	0.9900
C4—H4B	0.9900	C13—C14	1.372 (8)
C5—C6	1.513 (8)	C13—H13	0.9500
C5—H5A	0.9900	C14—C15	1.394 (6)
C5—H5B	0.9900	C14—H14	0.9500
C6—H6A	0.9900	C15—C14^{ii}	1.394 (6)
C6—H6B	0.9900	C15—C16	1.473 (11)
O21—C21	1.433 (9)	C16—C17	1.394 (7)
C21—C26	1.522 (10)	C16—C17^{ii}	1.394 (7)
C21—C22	1.522 (10)	C17—C18	1.378 (8)
C21—H21	1.0000	C17—H17	0.9500
C22—C23	1.510 (10)	C18—H18	0.9500
C22—H22A	0.9900		

N1—Ni—N2^{i}	180	H22A—C22—H22B	108.6
S1—Ni—S2	82.91 (5)	C24—C23—C22	111.0 (9)
S1—Ni—N1	91.41 (4)	C24—C23—H23A	109.4
S1—Ni—S1^{ii}	177.19 (8)	C22—C23—H23A	109.4
S1—Ni—S2^{ii}	97.17 (5)	C24—C23—H23B	109.4
S1—Ni—N2^{i}	88.59 (4)	C22—C23—H23B	109.4
S2—Ni—N1	88.33 (4)	H23A—C23—H23B	108.0
S2—Ni—S2^{ii}	176.66 (8)	C25—C24—C23	114.6 (10)
S2—Ni—N2^{i}	91.67 (4)	C25—C24—H24A	108.6
N1—Ni—S1^{ii}	91.41 (4)	C23—C24—H24A	108.6
N2^{i}—Ni—S1^{ii}	88.59 (4)	C25—C24—H24B	108.6
N2^{i}—Ni—S2^{ii}	91.67 (4)	C23—C24—H24B	108.6
S1^{ii}—Ni—S2^{ii}	82.91 (5)	H24A—C24—H24B	107.6
N1—Ni—S2	88.33 (4)	C24—C25—C26	109.4 (9)
S1^{ii}—Ni—S2	97.17 (5)	C24—C25—H25A	109.8
Ni—S1—P1	82.73 (6)	C26—C25—H25A	109.8
Ni—S2—P1	82.52 (7)	C24—C25—H25B	109.8
O2—P1—O21	99.6 (3)	C26—C25—H25B	109.8
O2—P1—O1	99.6 (3)	H25A—C25—H25B	108.2
O2—P1—S2	108.27 (16)	C21—C26—C25	104.4 (8)
O1—P1—S2	113.31 (17)	C21—C26—H26A	110.9
O2—P1—S1	112.08 (17)	C25—C26—H26A	110.9
O1—P1—S1	111.77 (19)	C21—C26—H26B	110.9
S2—P1—S1	111.26 (10)	C25—C26—H26B	110.9
C7—O2—P1	118.3 (4)	H26A—C26—H26B	108.9
C13—N1—C13^{ii}	116.7 (7)	O2—C7—C12	109.5 (6)
C13—N1—Ni	121.6 (3)	O2—C7—C8	108.9 (5)
C13^{ii}—N1—Ni	121.6 (3)	C12—C7—C8	113.1 (7)
C18—N2—C18^{ii}	116.1 (7)	O2—C7—H7	108.4
C18—N2—Ni^{iii}	121.9 (3)	C12—C7—H7	108.4
C18^{ii}—N2—Ni^{iii}	121.9 (3)	C8—C7—H7	108.4
C1—O1—P1	123.0 (4)	C7—C8—C9	110.4 (7)

O1—C1—C2	103.5 (6)	C7—C8—H8A	109.6
O1—C1—C6	105.5 (6)	C9—C8—H8A	109.6
C2—C1—C6	106.1 (6)	C7—C8—H8B	109.6
O1—C1—H1	113.6	C9—C8—H8B	109.6
C2—C1—H1	113.6	H8A—C8—H8B	108.1
C6—C1—H1	113.6	C10—C9—C8	111.4 (8)
C3—C2—C1	110.4 (7)	C10—C9—H9A	109.3
C3—C2—H2A	109.6	C8—C9—H9A	109.3
C1—C2—H2A	109.6	C10—C9—H9B	109.3
C3—C2—H2B	109.6	C8—C9—H9B	109.3
C1—C2—H2B	109.6	H9A—C9—H9B	108.0
H2A—C2—H2B	108.1	C9—C10—C11	110.7 (8)
C2—C3—C4	111.0 (6)	C9—C10—H10A	109.5
C2—C3—H3A	109.4	C11—C10—H10A	109.5
C4—C3—H3A	109.4	C9—C10—H10B	109.5
C2—C3—H3B	109.4	C11—C10—H10B	109.5
C4—C3—H3B	109.4	H10A—C10—H10B	108.1
H3A—C3—H3B	108.0	C10—C11—C12	112.0 (7)
C5—C4—C3	109.9 (6)	C10—C11—H11A	109.2
C5—C4—H4A	109.7	C12—C11—H11A	109.2
C3—C4—H4A	109.7	C10—C11—H11B	109.2
C5—C4—H4B	109.7	C12—C11—H11B	109.2
C3—C4—H4B	109.7	H11A—C11—H11B	107.9
H4A—C4—H4B	108.2	C7—C12—C11	108.8 (7)
C6—C5—C4	109.9 (6)	C7—C12—H12A	109.9
C6—C5—H5A	109.7	C11—C12—H12A	109.9
C4—C5—H5A	109.7	C7—C12—H12B	109.9
C6—C5—H5B	109.7	C11—C12—H12B	109.9
C4—C5—H5B	109.7	H12A—C12—H12B	108.3
H5A—C5—H5B	108.2	N1—C13—C14	123.3 (5)
C5—C6—C1	108.0 (6)	N1—C13—H13	118.3
C5—C6—H6A	110.1	C14—C13—H13	118.3
C1—C6—H6A	110.1	C13—C14—C15	120.2 (5)
C5—C6—H6B	110.1	C13—C14—H14	119.9
C1—C6—H6B	110.1	C15—C14—H14	119.9
H6A—C6—H6B	108.4	C14—C15—C14^{ii}	116.1 (7)
C21—O21—P1	123.0 (4)	C14—C15—C16	121.9 (3)
O21—C21—C26	131.5 (10)	C14^{ii}—C15—C16	121.9 (3)
O21—C21—C22	114.4 (12)	C17—C16—C17^{ii}	116.4 (7)
C26—C21—C22	108.0 (9)	C17—C16—C15	121.8 (4)
O21—C21—H21	98.1	C17^{ii}—C16—C15	121.8 (4)
C26—C21—H21	98.1	C18—C17—C16	120.0 (5)
C22—C21—H21	98.1	C18—C17—H17	120.0
C21—C22—C23	106.8 (9)	C16—C17—H17	120.0
C21—C22—H22A	110.4	C17—C18—N2	123.8 (5)
C23—C22—H22A	110.4	C17—C18—H18	118.1
C21—C22—H22B	110.4	N2—C18—H18	118.1
C23—C22—H22B	110.4		

N1—Ni—S1—P1	−93.16 (6)	O1—C1—C6—C5	−172.4 (8)
N2^{i}—Ni—S1—P1	86.84 (6)	C2—C1—C6—C5	−63.0 (11)
S2^{ii}—Ni—S1—P1	178.35 (7)	O2—P1—O21—C21	−169.9 (5)
S2—Ni—S1—P1	−5.02 (7)	S2—P1—O21—C21	75.3 (5)
N1—Ni—S2—P1	96.67 (6)	S1—P1—O21—C21	−51.4 (5)
N2^{i}—Ni—S2—P1	−83.33 (6)	P1—O21—C21—C26	−63.9 (11)
S1^{ii}—Ni—S2—P1	−172.12 (7)	P1—O21—C21—C22	147.4 (8)
S1—Ni—S2—P1	5.04 (7)	O21—C21—C22—C23	88.1 (15)
Ni—S2—P1—O2	116.91 (18)	C26—C21—C22—C23	−67.8 (16)
Ni—S2—P1—O21	−133.6 (2)	C21—C22—C23—C24	56 (2)
Ni—S2—P1—O1	−133.6 (2)	C22—C23—C24—C25	−51 (2)
Ni—S2—P1—S1	−6.67 (9)	C23—C24—C25—C26	54 (2)
Ni—S1—P1—O2	−114.68 (18)	O21—C21—C26—C25	−80.1 (15)
Ni—S1—P1—O21	134.49 (19)	C22—C21—C26—C25	70.1 (14)
Ni—S1—P1—O1	134.49 (19)	C24—C25—C26—C21	−61.4 (17)
Ni—S1—P1—S2	6.71 (9)	P1—O2—C7—C12	121.2 (6)
O21—P1—O2—C7	68.7 (5)	P1—O2—C7—C8	−114.7 (6)
O1—P1—O2—C7	68.7 (5)	O2—C7—C8—C9	−179.6 (7)
S2—P1—O2—C7	−172.7 (4)	C12—C7—C8—C9	−57.7 (9)
S1—P1—O2—C7	−49.7 (5)	C7—C8—C9—C10	56.3 (10)
S1^{ii}—Ni—N1—C13	−29.4 (3)	C8—C9—C10—C11	−56.1 (10)
S1—Ni—N1—C13	150.6 (3)	C9—C10—C11—C12	55.2 (11)
S2^{ii}—Ni—N1—C13	−112.2 (3)	O2—C7—C12—C11	177.2 (5)
S2—Ni—N1—C13	67.8 (3)	C8—C7—C12—C11	55.6 (8)
S1^{ii}—Ni—N1—C13^{ii}	150.6 (3)	C10—C11—C12—C7	−54.5 (11)
S1—Ni—N1—C13^{ii}	−29.4 (3)	C13^{ii}—N1—C13—C14	0.3 (5)
S2^{ii}—Ni—N1—C13^{ii}	67.8 (3)	Ni—N1—C13—C14	−179.7 (5)
S2—Ni—N1—C13^{ii}	−112.2 (3)	N1—C13—C14—C15	−0.6 (9)
O2—P1—O1—C1	−169.9 (5)	C13—C14—C15—C14^{ii}	0.3 (4)
S2—P1—O1—C1	75.3 (5)	C13—C14—C15—C16	−179.7 (4)
S1—P1—O1—C1	−51.4 (5)	C14—C15—C16—C17	−37.7 (4)
P1—O1—C1—C2	158.6 (6)	C14^{ii}—C15—C16—C17	142.3 (4)
P1—O1—C1—C6	−90.1 (7)	C14—C15—C16—C17^{ii}	142.3 (4)
O1—C1—C2—C3	172.3 (8)	C14^{ii}—C15—C16—C17^{ii}	−37.7 (4)
C6—C1—C2—C3	61.5 (12)	C17^{ii}—C16—C17—C18	0.1 (4)
C1—C2—C3—C4	−59.3 (12)	C15—C16—C17—C18	−179.9 (4)
C2—C3—C4—C5	56.8 (10)	C16—C17—C18—N2	−0.1 (8)
C3—C4—C5—C6	−59.2 (10)	C18^{ii}—N2—C18—C17	0.1 (4)
C4—C5—C6—C1	63.2 (11)	Ni^{iii}—N2—C18—C17	−179.9 (4)

Symmetry codes: (i) $x, y-1, z$; (ii) $-x, y, -z+1/2$; (iii) $x, y+1, z$.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···S2^{iv}	0.95	2.86	3.604 (5)	136

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