

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

catena-Poly[[bis(*O,O'*-diisopropyl dithiophosphato- κ^2 S,S')nickel(II)]- μ -bis(4-pyridylmethylene)diazane- κ^2 N:N']

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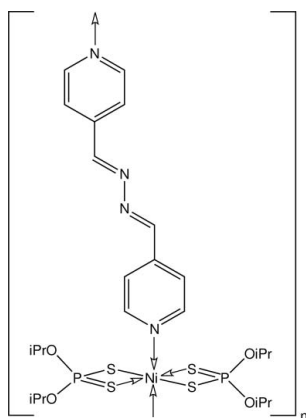
Received 21 October 2009; accepted 22 October 2009

Key indicators: single-crystal X-ray study; $T = 98$ K; mean $\sigma(\text{C}-\text{C}) = 0.004$ Å; R factor = 0.043; wR factor = 0.111; data-to-parameter ratio = 21.4.

The Ni atom in the title linear supramolecular polymer, $[\text{Ni}(\text{C}_6\text{H}_{14}\text{O}_2\text{PS}_2)_2(\text{C}_{12}\text{H}_{10}\text{N}_4)]_n$, exists within a *trans*- NiS_4 octahedral donor set defined by two symmetrically coordinating dithiophosphate ligands and pyridine N atoms derived from two bridging bis(4-pyridylmethylene)diazane ligands. The Ni atom lies on a centre of inversion and the bis(4-pyridylmethylene)diazane ligand is also disposed about a centre of inversion. The chains are arranged into layers sustained by $\text{C}-\text{H}\cdots\text{S}$ contacts and interdigitate with neighbouring layers, forming the crystal structure.

Related literature

For background to supramolecular polymers of metal dithiophosphates, see: Lai & Tiekink (2004); Chen *et al.* (2006); Aragoni *et al.* (2007). For a related *iso*-butyl structure and the synthesis, see: Berdugo & Tiekink (2008).



Experimental

Crystal data

$[\text{Ni}(\text{C}_6\text{H}_{14}\text{O}_2\text{PS}_2)_2(\text{C}_{12}\text{H}_{10}\text{N}_4)]$
 $M_r = 695.47$
 Triclinic, $P\bar{1}$
 $a = 8.661$ (2) Å
 $b = 8.753$ (2) Å
 $c = 11.159$ (3) Å
 $\alpha = 88.110$ (8)°
 $\beta = 81.502$ (7)°
 $\gamma = 89.813$ (10)°
 $V = 836.2$ (4) Å³
 $Z = 1$
 Mo $K\alpha$ radiation
 $\mu = 0.96$ mm⁻¹
 $T = 98$ K
 $0.50 \times 0.08 \times 0.05$ mm

Data collection

Rigaku AFC12K/SATURN724 diffractometer
 Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.794$, $T_{\max} = 1$
 7552 measured reflections
 3810 independent reflections
 3555 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.111$
 $S = 1.09$
 3810 reflections
 178 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.63$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.70$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

| | | | |
|----------|------------|-------|-------------|
| Ni—S1 | 2.4827 (7) | Ni—N1 | 2.1051 (19) |
| Ni—S2 | 2.4835 (7) | | |
| S1—Ni—S2 | 82.46 (2) | | |

Table 2

Hydrogen-bond geometry (Å, °).

| <i>D</i> —H \cdots <i>A</i> | <i>D</i> —H | H \cdots <i>A</i> | <i>D</i> \cdots <i>A</i> | <i>D</i> —H \cdots <i>A</i> |
|--------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C8—H8 \cdots S2 ⁱ | 0.95 | 2.77 | 3.694 (3) | 164 |

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

Data collection: *CrystalClear* (Rigaku/MSC 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *SHELXL97*.

The authors gratefully thank the MBRS–RISE program (GM60655) for support. Cheminova is also thanked for the gift of the dithiophosphate used in this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5163).

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supporting information

Acta Cryst. (2009). E65, m1444–m1445 [https://doi.org/10.1107/S1600536809043505]

***catena*-Poly[[bis(*O,O'*-diisopropyl dithiophosphato- κ^2 *S,S'*)nickel(II)]- μ -bis(4-pyridylmethylene)diazane- κ^2 *N:N'*]**

Erick Berdugo and Edward R. T. Tiekink

S1. Comment

Interest in molecules related to the title compound (I) revolve around intriguing crystal engineering possibilities whereby different supramolecular topologies may be constructed by careful choice of organic substituents and bridging ligands (Lai & Tiekink, 2004; Chen *et al.*, 2006; Aragoni *et al.*, 2007). The Ni atom in (I), Fig. 1, lies on a crystallographic centre of inversion and the bis(4-pyridylmethylene)diazane molecule is similarly disposed about a centre of inversion. The Ni atom exists within an octahedral *trans*-N₂S₄ donor set defined by two symmetrically chelating dithiophosphate ligands and two *trans*-disposed pyridine-N atoms, Table 1. The bridging ligands lead to a linear polymer, Fig. 2, and these are arranged into layers, being connected by C—H \cdots S contacts, Table 2 and Fig. 3. Layers interdigitate to consolidate the crystal packing, Fig. 4.

A similar coordination geometry and linear supramolecular polymer were observed in the iso-butyl derivative of (I) which was characterized crystallographically as a di-toluene solvate (Berdugo & Tiekink, 2008).

S2. Experimental

Compound (I) was prepared by refluxing the parent nickel dithiophosphate with bis(4-pyridylmethylene)diazane, following a literature procedure (Berdugo & Tiekink, 2008).

S3. Refinement

The H atoms were geometrically placed (C—H = 0.95–1.00 Å) and refined as riding with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{methyl-C})$.

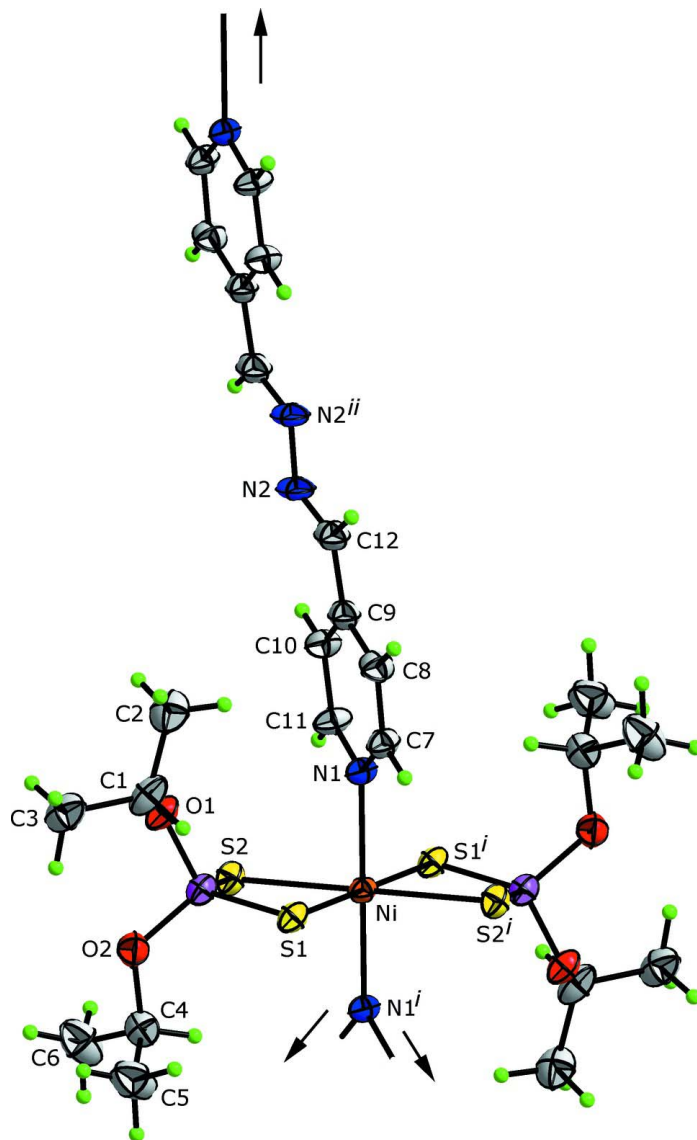


Figure 1

The asymmetric unit of (I) extended to show the Ni atom coordination geometry and a full molecule of the 4-pyridine-azine ligand, showing displacement ellipsoids at the 50% probability level. Symmetry operation i: $1 - x, 1 - y, 1 - z$ and ii: $1 + x, 1 + y, -1 + z$.



Figure 2

Supramolecular chain in (I) with base vector $[11\bar{1}]$.

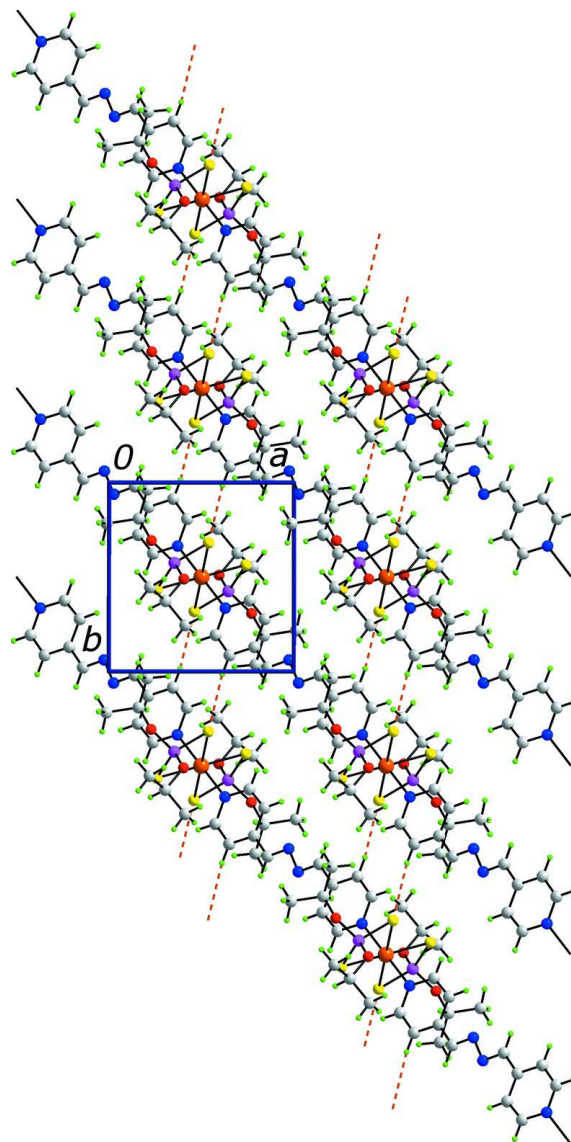


Figure 3

Layers of supramolecular chains mediated by C—H...S contacts (orange dashed lines), viewed in projection down the *c* axis.

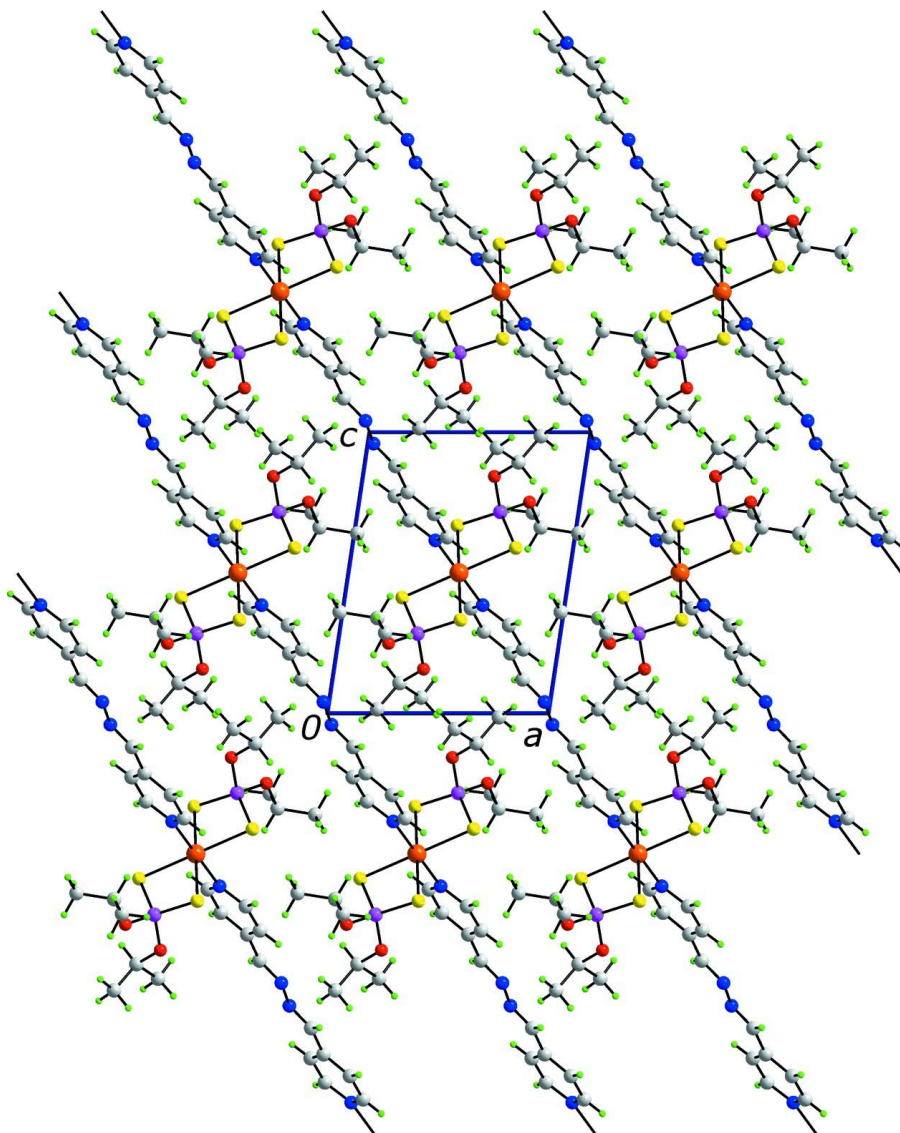


Figure 4

View of the interdigitation of layers in the crystal structure of (I), viewed in projection down the b axis.

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

Crystal data

$[\text{Ni}(\text{C}_6\text{H}_{14}\text{O}_2\text{PS}_2)_2(\text{C}_{12}\text{H}_{10}\text{N}_4)]$

$M_r = 695.47$

Triclinic, $P\bar{1}$

Hall symbol: $-P\ 1$

$a = 8.661(2)\ \text{\AA}$

$b = 8.753(2)\ \text{\AA}$

$c = 11.159(3)\ \text{\AA}$

$\alpha = 88.110(8)^\circ$

$\beta = 81.502(7)^\circ$

$\gamma = 89.813(10)^\circ$

$V = 836.2(4)\ \text{\AA}^3$

$Z = 1$

$F(000) = 364$

$D_x = 1.381\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71070\ \text{\AA}$

Cell parameters from 2817 reflections

$\theta = 3.0\text{--}32.3^\circ$

$\mu = 0.96\ \text{mm}^{-1}$

$T = 98\ \text{K}$

Prism, brown-orange

$0.50 \times 0.08 \times 0.05\ \text{mm}$

Data collection

Rigaku AFC12K/SATURN724
diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
 ω scans
Absorption correction: multi-scan
(*ABSCOR*; Higashi, 1995)
 $T_{\min} = 0.794$, $T_{\max} = 1$

7552 measured reflections
3810 independent reflections
3555 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.036$
 $\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.8^\circ$
 $h = -9 \rightarrow 11$
 $k = -11 \rightarrow 11$
 $l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.043$
 $wR(F^2) = 0.111$
 $S = 1.09$
3810 reflections
178 parameters
0 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
 $w = 1/[\sigma^2(F_o^2) + (0.0532P)^2 + 0.6278P]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$
 $\Delta\rho_{\max} = 0.63 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.70 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|-------------|--------------|--------------|----------------------------------|
| Ni | 0.5000 | 0.5000 | 0.5000 | 0.01506 (12) |
| S1 | 0.73976 (6) | 0.43573 (6) | 0.58844 (5) | 0.01900 (14) |
| S2 | 0.46123 (7) | 0.68201 (6) | 0.66788 (5) | 0.01887 (14) |
| P1 | 0.64607 (7) | 0.57524 (7) | 0.71650 (5) | 0.01822 (15) |
| O1 | 0.5953 (2) | 0.48949 (19) | 0.84272 (15) | 0.0223 (4) |
| O2 | 0.7711 (2) | 0.6930 (2) | 0.75100 (15) | 0.0241 (4) |
| N1 | 0.3710 (2) | 0.3357 (2) | 0.61516 (17) | 0.0177 (4) |
| N2 | 0.0259 (2) | 0.0611 (2) | 0.95949 (18) | 0.0230 (4) |
| C1 | 0.6944 (3) | 0.3733 (3) | 0.8926 (2) | 0.0261 (5) |
| H1 | 0.7730 | 0.3345 | 0.8257 | 0.031* |
| C2 | 0.5865 (3) | 0.2446 (3) | 0.9442 (2) | 0.0315 (6) |
| H2A | 0.5378 | 0.2009 | 0.8792 | 0.047* |
| H2B | 0.5053 | 0.2840 | 1.0061 | 0.047* |
| H2C | 0.6464 | 0.1653 | 0.9810 | 0.047* |
| C3 | 0.7778 (3) | 0.4463 (3) | 0.9858 (2) | 0.0305 (6) |
| H3A | 0.8473 | 0.5272 | 0.9464 | 0.046* |

| | | | | |
|-----|------------|------------|------------|------------|
| H3B | 0.8393 | 0.3688 | 1.0230 | 0.046* |
| H3C | 0.7009 | 0.4903 | 1.0486 | 0.046* |
| C4 | 0.8388 (3) | 0.8094 (3) | 0.6614 (2) | 0.0266 (5) |
| H4 | 0.7952 | 0.7981 | 0.5840 | 0.032* |
| C5 | 1.0132 (3) | 0.7830 (3) | 0.6398 (3) | 0.0384 (7) |
| H5A | 1.0350 | 0.6822 | 0.6055 | 0.058* |
| H5B | 1.0544 | 0.7876 | 0.7168 | 0.058* |
| H5C | 1.0634 | 0.8621 | 0.5831 | 0.058* |
| C6 | 0.7934 (3) | 0.9641 (3) | 0.7138 (3) | 0.0380 (7) |
| H6A | 0.6795 | 0.9747 | 0.7249 | 0.057* |
| H6B | 0.8410 | 1.0454 | 0.6581 | 0.057* |
| H6C | 0.8303 | 0.9718 | 0.7923 | 0.057* |
| C7 | 0.4224 (3) | 0.1924 (3) | 0.6265 (2) | 0.0198 (4) |
| H7 | 0.5144 | 0.1624 | 0.5755 | 0.024* |
| C8 | 0.3473 (3) | 0.0860 (3) | 0.7094 (2) | 0.0210 (5) |
| H8 | 0.3865 | -0.0153 | 0.7138 | 0.025* |
| C9 | 0.2132 (3) | 0.1289 (3) | 0.7867 (2) | 0.0194 (4) |
| C10 | 0.1577 (3) | 0.2772 (3) | 0.7726 (2) | 0.0212 (5) |
| H10 | 0.0653 | 0.3102 | 0.8217 | 0.025* |
| C11 | 0.2384 (3) | 0.3754 (3) | 0.6868 (2) | 0.0208 (5) |
| H11 | 0.1990 | 0.4758 | 0.6775 | 0.025* |
| C12 | 0.1396 (3) | 0.0206 (3) | 0.8798 (2) | 0.0225 (5) |
| H12 | 0.1765 | -0.0817 | 0.8815 | 0.027* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| Ni | 0.0173 (2) | 0.0127 (2) | 0.0143 (2) | 0.00009 (15) | 0.00006 (15) | 0.00119 (14) |
| S1 | 0.0197 (3) | 0.0198 (3) | 0.0170 (3) | 0.0034 (2) | -0.0009 (2) | -0.0008 (2) |
| S2 | 0.0208 (3) | 0.0174 (3) | 0.0183 (3) | 0.0039 (2) | -0.0023 (2) | -0.0019 (2) |
| P1 | 0.0192 (3) | 0.0193 (3) | 0.0158 (3) | 0.0020 (2) | -0.0015 (2) | -0.0011 (2) |
| O1 | 0.0243 (8) | 0.0249 (8) | 0.0174 (8) | 0.0055 (7) | -0.0025 (6) | 0.0016 (6) |
| O2 | 0.0240 (9) | 0.0279 (9) | 0.0209 (9) | -0.0010 (7) | -0.0045 (7) | -0.0036 (7) |
| N1 | 0.0182 (9) | 0.0170 (9) | 0.0165 (9) | -0.0004 (7) | 0.0013 (7) | 0.0017 (7) |
| N2 | 0.0238 (10) | 0.0212 (10) | 0.0223 (11) | -0.0065 (8) | 0.0006 (8) | 0.0090 (8) |
| C1 | 0.0270 (12) | 0.0323 (13) | 0.0186 (12) | 0.0112 (10) | -0.0032 (10) | 0.0033 (9) |
| C2 | 0.0412 (15) | 0.0265 (13) | 0.0280 (14) | 0.0055 (11) | -0.0096 (11) | 0.0026 (10) |
| C3 | 0.0256 (13) | 0.0412 (15) | 0.0250 (13) | 0.0024 (11) | -0.0059 (10) | 0.0051 (11) |
| C4 | 0.0274 (12) | 0.0259 (12) | 0.0266 (13) | -0.0038 (10) | -0.0034 (10) | -0.0033 (10) |
| C5 | 0.0279 (14) | 0.0344 (15) | 0.0503 (19) | -0.0032 (12) | 0.0044 (12) | -0.0087 (13) |
| C6 | 0.0298 (14) | 0.0289 (14) | 0.056 (2) | 0.0019 (11) | -0.0081 (13) | -0.0088 (13) |
| C7 | 0.0222 (11) | 0.0181 (10) | 0.0184 (11) | 0.0002 (9) | -0.0008 (9) | 0.0019 (8) |
| C8 | 0.0240 (11) | 0.0155 (10) | 0.0233 (12) | 0.0003 (9) | -0.0028 (9) | 0.0013 (8) |
| C9 | 0.0193 (11) | 0.0199 (11) | 0.0191 (11) | -0.0027 (8) | -0.0040 (8) | 0.0028 (8) |
| C10 | 0.0198 (11) | 0.0209 (11) | 0.0210 (12) | -0.0004 (9) | 0.0023 (9) | 0.0019 (9) |
| C11 | 0.0209 (11) | 0.0184 (10) | 0.0213 (12) | 0.0023 (9) | 0.0020 (9) | 0.0049 (8) |
| C12 | 0.0229 (11) | 0.0224 (11) | 0.0228 (12) | -0.0046 (9) | -0.0062 (9) | 0.0056 (9) |

Geometric parameters (Å, °)

| | | | |
|-------------------------------------|-------------|------------|-----------|
| Ni—S1 | 2.4827 (7) | C3—H3A | 0.9800 |
| Ni—S2 | 2.4835 (7) | C3—H3B | 0.9800 |
| Ni—N1 | 2.1051 (19) | C3—H3C | 0.9800 |
| Ni—N1 ⁱ | 2.1051 (19) | C4—C5 | 1.513 (4) |
| Ni—S1 ⁱ | 2.4827 (7) | C4—C6 | 1.520 (4) |
| Ni—S2 ⁱ | 2.4835 (7) | C4—H4 | 1.0000 |
| S1—P1 | 1.9895 (9) | C5—H5A | 0.9800 |
| S2—P1 | 1.9859 (9) | C5—H5B | 0.9800 |
| P1—O1 | 1.5779 (17) | C5—H5C | 0.9800 |
| P1—O2 | 1.5934 (18) | C6—H6A | 0.9800 |
| O1—C1 | 1.476 (3) | C6—H6B | 0.9800 |
| O2—C4 | 1.464 (3) | C6—H6C | 0.9800 |
| N1—C7 | 1.338 (3) | C7—C8 | 1.384 (3) |
| N1—C11 | 1.350 (3) | C7—H7 | 0.9500 |
| N2—C12 | 1.283 (3) | C8—C9 | 1.399 (3) |
| N2—N2 ⁱⁱ | 1.408 (4) | C8—H8 | 0.9500 |
| C1—C2 | 1.510 (4) | C9—C10 | 1.395 (3) |
| C1—C3 | 1.511 (4) | C9—C12 | 1.459 (3) |
| C1—H1 | 1.0000 | C10—C11 | 1.377 (3) |
| C2—H2A | 0.9800 | C10—H10 | 0.9500 |
| C2—H2B | 0.9800 | C11—H11 | 0.9500 |
| C2—H2C | 0.9800 | C12—H12 | 0.9500 |
| | | | |
| N1—Ni—S1 ⁱ | 89.02 (6) | C1—C3—H3B | 109.5 |
| N1 ⁱ —Ni—S1 ⁱ | 90.98 (6) | H3A—C3—H3B | 109.5 |
| N1—Ni—S1 | 90.98 (6) | C1—C3—H3C | 109.5 |
| N1 ⁱ —Ni—S1 | 89.02 (6) | H3A—C3—H3C | 109.5 |
| N1—Ni—S2 ⁱ | 91.02 (6) | H3B—C3—H3C | 109.5 |
| N1 ⁱ —Ni—S2 ⁱ | 88.98 (6) | O2—C4—C5 | 107.1 (2) |
| S1 ⁱ —Ni—S2 ⁱ | 82.46 (2) | O2—C4—C6 | 107.0 (2) |
| S1—Ni—S2 ⁱ | 97.54 (2) | C5—C4—C6 | 113.4 (2) |
| N1—Ni—S2 | 88.98 (6) | O2—C4—H4 | 109.8 |
| N1 ⁱ —Ni—S2 | 91.02 (6) | C5—C4—H4 | 109.8 |
| S1 ⁱ —Ni—S2 | 97.54 (2) | C6—C4—H4 | 109.8 |
| S1—Ni—S2 | 82.46 (2) | C4—C5—H5A | 109.5 |
| S1 ⁱ —Ni—S1 | 180.0 | C4—C5—H5B | 109.5 |
| S2 ⁱ —Ni—S2 | 180.0 | H5A—C5—H5B | 109.5 |
| N1 ⁱ —Ni—N1 | 180.0 | C4—C5—H5C | 109.5 |
| P1—S1—Ni | 82.80 (3) | H5A—C5—H5C | 109.5 |
| P1—S2—Ni | 82.85 (3) | H5B—C5—H5C | 109.5 |
| O1—P1—O2 | 100.84 (10) | C4—C6—H6A | 109.5 |
| O1—P1—S2 | 108.61 (7) | C4—C6—H6B | 109.5 |
| O2—P1—S2 | 111.61 (7) | H6A—C6—H6B | 109.5 |
| O1—P1—S1 | 112.72 (7) | C4—C6—H6C | 109.5 |
| O2—P1—S1 | 111.82 (7) | H6A—C6—H6C | 109.5 |
| S2—P1—S1 | 110.84 (4) | H6B—C6—H6C | 109.5 |

| | | | |
|---------------------------|--------------|-----------------------------|--------------|
| C1—O1—P1 | 122.47 (15) | N1—C7—C8 | 122.9 (2) |
| C4—O2—P1 | 119.75 (15) | N1—C7—H7 | 118.6 |
| C7—N1—C11 | 117.73 (19) | C8—C7—H7 | 118.6 |
| C7—N1—Ni | 121.63 (15) | C7—C8—C9 | 119.4 (2) |
| C11—N1—Ni | 120.48 (15) | C7—C8—H8 | 120.3 |
| C12—N2—N2 ⁱⁱ | 111.3 (2) | C9—C8—H8 | 120.3 |
| O1—C1—C2 | 106.2 (2) | C10—C9—C8 | 117.6 (2) |
| O1—C1—C3 | 108.7 (2) | C10—C9—C12 | 122.7 (2) |
| C2—C1—C3 | 113.5 (2) | C8—C9—C12 | 119.7 (2) |
| O1—C1—H1 | 109.5 | C11—C10—C9 | 119.2 (2) |
| C2—C1—H1 | 109.5 | C11—C10—H10 | 120.4 |
| C3—C1—H1 | 109.5 | C9—C10—H10 | 120.4 |
| C1—C2—H2A | 109.5 | N1—C11—C10 | 123.1 (2) |
| C1—C2—H2B | 109.5 | N1—C11—H11 | 118.4 |
| H2A—C2—H2B | 109.5 | C10—C11—H11 | 118.4 |
| C1—C2—H2C | 109.5 | N2—C12—C9 | 121.1 (2) |
| H2A—C2—H2C | 109.5 | N2—C12—H12 | 119.4 |
| H2B—C2—H2C | 109.5 | C9—C12—H12 | 119.4 |
| C1—C3—H3A | 109.5 | | |
| | | | |
| N1—Ni—S1—P1 | -82.10 (6) | S2—Ni—N1—C7 | -131.96 (18) |
| N1 ⁱ —Ni—S1—P1 | 97.90 (6) | S1 ⁱ —Ni—N1—C11 | -54.34 (18) |
| S2 ⁱ —Ni—S1—P1 | -173.26 (3) | S1—Ni—N1—C11 | 125.66 (18) |
| S2—Ni—S1—P1 | 6.74 (3) | S2 ⁱ —Ni—N1—C11 | -136.78 (18) |
| N1—Ni—S2—P1 | 84.37 (6) | S2—Ni—N1—C11 | 43.22 (18) |
| N1 ⁱ —Ni—S2—P1 | -95.63 (6) | P1—O1—C1—C2 | -137.26 (18) |
| S1 ⁱ —Ni—S2—P1 | 173.24 (3) | P1—O1—C1—C3 | 100.3 (2) |
| S1—Ni—S2—P1 | -6.76 (3) | P1—O2—C4—C5 | -119.8 (2) |
| Ni—S2—P1—O1 | -115.40 (7) | P1—O2—C4—C6 | 118.37 (19) |
| Ni—S2—P1—O2 | 134.30 (7) | C11—N1—C7—C8 | -1.3 (3) |
| Ni—S2—P1—S1 | 8.96 (3) | Ni—N1—C7—C8 | 174.02 (18) |
| Ni—S1—P1—O1 | 113.02 (8) | N1—C7—C8—C9 | -1.1 (4) |
| Ni—S1—P1—O2 | -134.19 (7) | C7—C8—C9—C10 | 2.6 (3) |
| Ni—S1—P1—S2 | -8.96 (3) | C7—C8—C9—C12 | -175.8 (2) |
| O2—P1—O1—C1 | -75.87 (19) | C8—C9—C10—C11 | -1.8 (3) |
| S2—P1—O1—C1 | 166.73 (16) | C12—C9—C10—C11 | 176.6 (2) |
| S1—P1—O1—C1 | 43.51 (19) | C7—N1—C11—C10 | 2.1 (4) |
| O1—P1—O2—C4 | -173.76 (16) | Ni—N1—C11—C10 | -173.22 (18) |
| S2—P1—O2—C4 | -58.58 (17) | C9—C10—C11—N1 | -0.6 (4) |
| S1—P1—O2—C4 | 66.22 (17) | N2 ⁱⁱ —N2—C12—C9 | -179.5 (2) |
| S1 ⁱ —Ni—N1—C7 | 130.48 (18) | C10—C9—C12—N2 | -5.2 (4) |
| S1—Ni—N1—C7 | -49.52 (18) | C8—C9—C12—N2 | 173.1 (2) |
| S2 ⁱ —Ni—N1—C7 | 48.04 (18) | | |

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

Hydrogen-bond geometry (\AA , $^\circ$)

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------|-------|-------------|-------------|---------------|
| $C8-H8\cdots S2^{iii}$ | 0.95 | 2.77 | 3.694 (3) | 164 |

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