# Bis[*O*-methyl (4-ethoxyphenyl)dithiophosphonato-$\kappa^2S,S'$]nickel(II)

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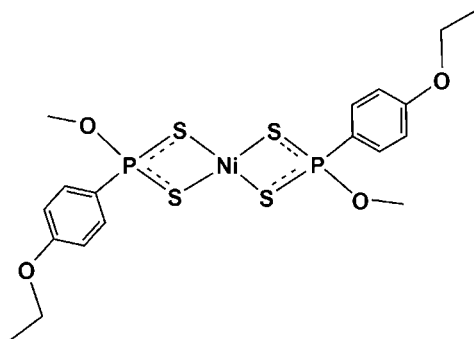Correspondence e-mail: vanzylw@ukzn.ac.za

In the title compound, [Ni($C_9H_{12}O_2PS_2$)$_2$], the Ni$^{II}$ atom resides on an inversion center and is coordinated by four S atoms [Ni—S = 2.2328 (4) and 2.2455 (3) Å] in a distorted square-planar geometry [S—Ni—S = 88.443 (13) and 91.557 (13)°]. In the crystal, molecules related by translation in [110] are linked into chains *via* weak C—H⋯O interactions. The crystal packing exhibits short intermolecular S⋯S contacts of 3.3366 (5) Å.

## Related literature

For information on dithiophosphonate compounds, see: Van Zyl & Fackler (2000); Van Zyl (2010); Van Zyl & Woollins (2012). For related structures of nickel(II) dithiophosphonate complexes, see: Hartung (1967); Liu *et al.* (2004); Gray *et al.* (2004); Aragoni *et al.* (2007); Arca *et al.* (1997); Özcan *et al.* (2002).



## Experimental

### Crystal data

[Ni($C_9H_{12}O_2PS_2$)$_2$]
$M_r$ = 553.26
Monoclinic, $P2_1/c$
$a$ = 13.5866 (5) Å
$b$ = 6.4212 (2) Å
$c$ = 14.1047 (5) Å
$\beta$ = 109.389 (2)°
$V$ = 1160.74 (7) Å³
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.36 mm$^{-1}$
$T$ = 173 K
$0.43 \times 0.31 \times 0.24$ mm

### Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
$T_{min}$ = 0.593, $T_{max}$ = 0.737
19824 measured reflections
2850 independent reflections
2609 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.036

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.062
$S$ = 1.07
2850 reflections
135 parameters
2 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.56 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.44 e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| $D$—H⋯$A$ | $D$—H | H⋯$A$ | $D$⋯$A$ | $D$—H⋯$A$ |
|---|---|---|---|---|
| C3—H3⋯O1$^i$ | 0.95 | 2.57 | 3.5123 (18) | 171 |

Symmetry code: (i) $-x + 1, -y + 1, -z + 2$.

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT-Plus* (Bruker, 2008); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2008); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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# supporting information

# Bis[*O*-methyl (4-ethoxyphenyl)dithiophosphonato-*κ²S,S′*]nickel(II)

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### S1. Comment

The phosphor-1,1-dithiolate class of compounds is the heavier and softer congener of the popular phosphonate derivatives. It contains the $S_2P$ functionality as a common feature and several sub-categories are known which include the dithiophosphato $[S_2P(OR)_2]^-$, (*R* = typically alkyl), dithiophosphinato $[S_2PR_2]^-$ (*R* = alkyl or aryl), and dithiophosphonato $[S_2PR(OR′)]^-$, (*R* = typically aryl or ferrocenyl, *R′* = alkyl) monoanionic ligands. The latter may be described as a hybrid of the former two, and are also much less developed. Amongst all metals involved in the coordination chemistry of dithiophosphonato ligands, however, nickel(II) is by far the best represented (Van Zyl & Woollins, 2012) with the first X-ray structural report of a nickel(II) dithiophosphonate complex reported more than four decades ago (Hartung, 1967). The title complex, (I), was formed from the reaction between $NiCl_2.6H_20$ and the ammonium salt of $[S_2P(OMe)(4-C_6H_4OEt)]$ (molar ratio 1:2) in an aqueous/methanolic solution, the $NH_4Cl$ by-product was dissolved and the precipitated product filtered off and washed with water. General and convenient methods to prepare dithiophosphonate salt derivatives have been reported (Van Zyl & Fackler, 2000).

The structure of (I) (Fig. 1) does not differ significantly from related Ni(II) complexes previously reported (Aragoni *et al.*, 2007; Arca *et al.* (1997); Gray *et al.* (2004); Liu *et al.* (2004); Özcan *et al.*, 2002). The Ni atom in (I) resides on an inversion center and is coordinated by four S atoms [Ni—S 2.2328 (4), 2.2455 (3) Å] in a distorted square-planar geometry [S—Ni—S 88.443 (13), 91.557 (13)°]. Molecules related by translation in [110] are linked into chains *via* weak C—H···O interactions (Table 1). The crystal packing exhibits short intermolecular S···S contacts of 3.3366 (5) Å.

### S2. Experimental

A colorless methanol (40 ml) solution of $NH_4[S_2P(OMe)(4-C_6H_4OEt)]$ (1.044 g, 4.474 mmol) was prepared. A second green solution of $NiCl_2.6H_20$ (540 mg, 2.272 mmol) in deionized water (20 ml) was prepared, and added to the colorless solution with stirring over a period of 5 min. This resulted in a purple precipitate indicating the formation of the title complex. The precipitate was collected by vacuum filtration, washed with water (3 *x* 10 ml) and allowed to dry under vacuum for a period of 3 hrs, yielding a dry, free-flowing purple powder. Purple crystals suitable for X-ray analysis were grown by the slow diffusion of hexane into a dichloromethane solution of the title complex. Yield: 1.004 g, 41%. *M*.p. 168°C.

$^{31}P$ NMR (CDCl$_3$): $\delta$ (p.p.m.): 104.56. $^1H$ NMR (CDCl$_3$): $\delta$ (p.p.m.): 7.94 (2*H*, dd, J($^{31}P$-$^1H$) = 12.76 Hz, J($^1H$ -$^1H$) = 10.08 Hz, *o*-ArH), 6.95 (2*H*, dd, J($^{31}P$-$^1H$) = 8.76 Hz, J($^1H$-$^1H$) = 3.08 Hz, *m*-ArH), 4.07 (2*H*, quart, J($^1H$-$^1H$) = 6.96 Hz, ArOCH$_2$), 3.96 (3*H*, d, J($^{31}P$-$^1H$) = 14.8 Hz, POCH$_3$), 1.41 (3*H*, t, J($^1H$-$^1H$) = 6.98 Hz, ArOCH$_2$CH$_3$). $^{13}C$ NMR (CDCl$_3$): $\delta$ (p.p.m.): 162.64 (*p*-ArC), 131.78 (*m*-ArC), 128.68 (Ar—C$_{ipso}$), 114.62 (*o*-ArC), 63.99 (ArOCH$_2$), 52.73 (OCH$_3$), 14.85 (ArOCH$_2$CH$_3$).

## S3. Refinement

All hydrogen atoms were found in the difference electron density maps, then placed in idealized positions (C—H = 0.95–1.00 Å) and refined as riding, with $U_{iso}(H)$ = 1.2-1.5 $U_{eq}(C)$.
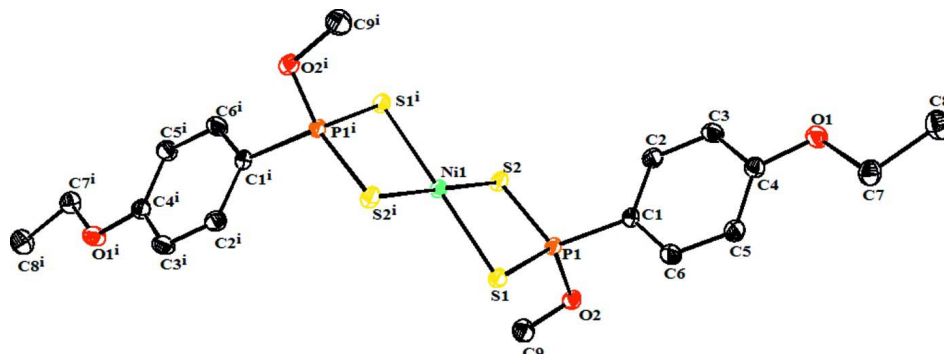


**Figure 1**

The molecular structure of the title complex showing the atomic numbering and 50% probability displacement ellipsoids [symmetry code: (i)-$x$ + 2,-$y$ + 2,-$z$ + 2]. H atoms omitted for clarity.

**Bis[*O*-methyl (4-ethoxyphenyl)dithiophosphonato- $\kappa^2 S, S'$]nickel(II)**

*Crystal data*

| | |
|---|---|
| [Ni(C₉H₁₂O₂PS₂)₂] | $F(000)$ = 572 |
| $M_r$ = 553.26 | $D_x$ = 1.583 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å |
| Hall symbol: -P 2ybc | Cell parameters from 19824 reflections |
| $a$ = 13.5866 (5) Å | $\theta$ = 2.9–28.4° |
| $b$ = 6.4212 (2) Å | $\mu$ = 1.36 mm$^{-1}$ |
| $c$ = 14.1047 (5) Å | $T$ = 173 K |
| $\beta$ = 109.389 (2)° | Block, purple |
| $V$ = 1160.74 (7) Å³ | 0.43 × 0.31 × 0.24 mm |
| $Z$ = 2 | |

*Data collection*

| | |
|---|---|
| Bruker SMART APEXII CCD diffractometer | 19824 measured reflections |
| Radiation source: fine-focus sealed tube | 2850 independent reflections |
| Graphite monochromator | 2609 reflections with $I > 2\sigma(I)$ |
| $\varphi$ and $\omega$ scans | $R_{int}$ = 0.036 |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2008) | $\theta_{max}$ = 28.4°, $\theta_{min}$ = 2.9° |
| | $h$ = −18→17 |
| | $k$ = −8→8 |
| $T_{min}$ = 0.593, $T_{max}$ = 0.737 | $l$ = −18→18 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)]$ = 0.023 | |
| $wR(F^2)$ = 0.062 | Hydrogen site location: inferred from neighbouring sites |
| $S$ = 1.07 | |
| 2850 reflections | H-atom parameters constrained |
| 135 parameters | |
| 2 restraints | |

$w = 1/[\sigma^2(F_o^2) + (0.0281P)^2 + 0.7956P]$
  where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.56$ e Å⁻³
$\Delta\rho_{min} = -0.44$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.70393 (11) | 0.8288 (2) | 0.85131 (10) | 0.0149 (3) |
| C2 | 0.68704 (11) | 0.6590 (2) | 0.90614 (11) | 0.0175 (3) |
| H2 | 0.7398 | 0.5564 | 0.9306 | 0.021* |
| C3 | 0.59371 (12) | 0.6398 (2) | 0.92488 (12) | 0.0196 (3) |
| H3 | 0.5823 | 0.5237 | 0.9617 | 0.024* |
| C4 | 0.51619 (11) | 0.7913 (2) | 0.88969 (11) | 0.0167 (3) |
| C5 | 0.53108 (12) | 0.9588 (3) | 0.83320 (12) | 0.0202 (3) |
| H5 | 0.4777 | 1.0598 | 0.8075 | 0.024* |
| C6 | 0.62531 (12) | 0.9759 (3) | 0.81507 (12) | 0.0211 (3) |
| H6 | 0.6362 | 1.0905 | 0.7771 | 0.025* |
| C7 | 0.34352 (11) | 0.9068 (2) | 0.87693 (12) | 0.0199 (3) |
| H7A | 0.3191 | 0.9120 | 0.8026 | 0.024* |
| H7B | 0.3662 | 1.0480 | 0.9033 | 0.024* |
| C8 | 0.25769 (12) | 0.8303 (3) | 0.91356 (13) | 0.0258 (3) |
| H8A | 0.2401 | 0.6862 | 0.8915 | 0.039* |
| H8B | 0.1959 | 0.9186 | 0.8859 | 0.039* |
| H8C | 0.2812 | 0.8364 | 0.9871 | 0.039* |
| C9 | 0.88481 (12) | 0.8281 (3) | 0.67579 (12) | 0.0243 (3) |
| H9A | 0.9184 | 0.9650 | 0.6891 | 0.036* |
| H9B | 0.8562 | 0.8052 | 0.6031 | 0.036* |
| H9C | 0.9363 | 0.7197 | 0.7065 | 0.036* |
| O1 | 0.42818 (8) | 0.76065 (18) | 0.91366 (8) | 0.0210 (2) |
| O2 | 0.80067 (8) | 0.81965 (17) | 0.71841 (7) | 0.0172 (2) |
| P1 | 0.82716 (3) | 0.87053 (6) | 0.83456 (3) | 0.01290 (9) |
| S1 | 0.88018 (3) | 1.16115 (5) | 0.87163 (3) | 0.01505 (9) |
| S2 | 0.94269 (3) | 0.69659 (5) | 0.92450 (3) | 0.01547 (9) |
| Ni1 | 1.0000 | 1.0000 | 1.0000 | 0.01236 (8) |

*Atomic displacement parameters (Å²)*

|  | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0126 (6) | 0.0163 (7) | 0.0142 (6) | −0.0026 (5) | 0.0024 (5) | −0.0008 (5) |

| | | | | | |
|---|---|---|---|---|---|
| C2 | 0.0168 (7) | 0.0162 (7) | 0.0186 (7) | 0.0021 (5) | 0.0050 (5) | 0.0025 (6) |
| C3 | 0.0200 (7) | 0.0181 (7) | 0.0218 (7) | 0.0007 (6) | 0.0085 (6) | 0.0061 (6) |
| C4 | 0.0156 (6) | 0.0187 (7) | 0.0157 (6) | −0.0013 (6) | 0.0050 (5) | −0.0007 (6) |
| C5 | 0.0152 (7) | 0.0194 (7) | 0.0246 (7) | 0.0024 (6) | 0.0050 (6) | 0.0065 (6) |
| C6 | 0.0177 (7) | 0.0201 (7) | 0.0252 (7) | 0.0005 (6) | 0.0067 (6) | 0.0088 (6) |
| C7 | 0.0171 (7) | 0.0192 (7) | 0.0239 (7) | 0.0027 (6) | 0.0074 (6) | −0.0006 (6) |
| C8 | 0.0209 (7) | 0.0271 (9) | 0.0324 (9) | 0.0015 (6) | 0.0127 (7) | −0.0004 (7) |
| C9 | 0.0219 (7) | 0.0328 (9) | 0.0212 (7) | 0.0004 (7) | 0.0113 (6) | −0.0025 (7) |
| O1 | 0.0176 (5) | 0.0231 (6) | 0.0251 (5) | 0.0041 (4) | 0.0107 (4) | 0.0069 (5) |
| O2 | 0.0164 (5) | 0.0212 (5) | 0.0133 (5) | −0.0019 (4) | 0.0038 (4) | −0.0016 (4) |
| P1 | 0.01195 (16) | 0.01266 (17) | 0.01283 (16) | −0.00089 (13) | 0.00241 (13) | 0.00025 (13) |
| S1 | 0.01442 (16) | 0.01179 (16) | 0.01655 (16) | −0.00085 (12) | 0.00194 (13) | 0.00125 (13) |
| S2 | 0.01453 (16) | 0.01163 (17) | 0.01733 (16) | 0.00058 (12) | 0.00138 (13) | −0.00038 (13) |
| Ni1 | 0.01162 (12) | 0.01061 (13) | 0.01350 (12) | −0.00046 (9) | 0.00235 (9) | 0.00017 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C6 | 1.390 (2) | C8—H8A | 0.9800 |
| C1—C2 | 1.399 (2) | C8—H8B | 0.9800 |
| C1—P1 | 1.7871 (14) | C8—H8C | 0.9800 |
| C2—C3 | 1.384 (2) | C9—O2 | 1.4585 (17) |
| C2—H2 | 0.9500 | C9—H9A | 0.9800 |
| C3—C4 | 1.398 (2) | C9—H9B | 0.9800 |
| C3—H3 | 0.9500 | C9—H9C | 0.9800 |
| C4—O1 | 1.3606 (17) | O2—P1 | 1.5902 (10) |
| C4—C5 | 1.393 (2) | P1—S2 | 1.9996 (5) |
| C5—C6 | 1.391 (2) | P1—S1 | 2.0061 (5) |
| C5—H5 | 0.9500 | P1—Ni1 | 2.8306 (4) |
| C6—H6 | 0.9500 | S1—Ni1 | 2.2455 (3) |
| C7—O1 | 1.4408 (18) | S2—Ni1 | 2.2328 (4) |
| C7—C8 | 1.506 (2) | Ni1—S2ⁱ | 2.2328 (4) |
| C7—H7A | 0.9900 | Ni1—S1ⁱ | 2.2455 (3) |
| C7—H7B | 0.9900 | Ni1—P1ⁱ | 2.8306 (4) |
| | | | |
| C6—C1—C2 | 119.07 (13) | O2—C9—H9C | 109.5 |
| C6—C1—P1 | 119.25 (11) | H9A—C9—H9C | 109.5 |
| C2—C1—P1 | 121.52 (11) | H9B—C9—H9C | 109.5 |
| C3—C2—C1 | 120.23 (14) | C4—O1—C7 | 118.63 (12) |
| C3—C2—H2 | 119.9 | C9—O2—P1 | 118.47 (9) |
| C1—C2—H2 | 119.9 | O2—P1—C1 | 101.76 (6) |
| C2—C3—C4 | 120.03 (14) | O2—P1—S2 | 113.60 (4) |
| C2—C3—H3 | 120.0 | C1—P1—S2 | 113.88 (5) |
| C4—C3—H3 | 120.0 | O2—P1—S1 | 113.49 (4) |
| O1—C4—C5 | 124.08 (14) | C1—P1—S1 | 112.10 (5) |
| O1—C4—C3 | 115.59 (13) | S2—P1—S1 | 102.47 (2) |
| C5—C4—C3 | 120.33 (13) | O2—P1—Ni1 | 138.74 (4) |
| C6—C5—C4 | 118.91 (14) | C1—P1—Ni1 | 119.49 (5) |
| C6—C5—H5 | 120.5 | S2—P1—Ni1 | 51.639 (13) |

| | | | |
|---|---|---|---|
| C4—C5—H5 | 120.5 | S1—P1—Ni1 | 51.985 (12) |
| C1—C6—C5 | 121.39 (14) | P1—S1—Ni1 | 83.279 (16) |
| C1—C6—H6 | 119.3 | P1—S2—Ni1 | 83.755 (17) |
| C5—C6—H6 | 119.3 | S2^i—Ni1—S2 | 180.0 |
| O1—C7—C8 | 106.33 (13) | S2^i—Ni1—S1 | 91.557 (13) |
| O1—C7—H7A | 110.5 | S2—Ni1—S1 | 88.443 (13) |
| C8—C7—H7A | 110.5 | S2^i—Ni1—S1^i | 88.443 (13) |
| O1—C7—H7B | 110.5 | S2—Ni1—S1^i | 91.557 (13) |
| C8—C7—H7B | 110.5 | S1—Ni1—S1^i | 180.0 |
| H7A—C7—H7B | 108.7 | S2^i—Ni1—P1^i | 44.606 (11) |
| C7—C8—H8A | 109.5 | S2—Ni1—P1^i | 135.394 (11) |
| C7—C8—H8B | 109.5 | S1—Ni1—P1^i | 135.263 (12) |
| H8A—C8—H8B | 109.5 | S1^i—Ni1—P1^i | 44.737 (12) |
| C7—C8—H8C | 109.5 | S2^i—Ni1—P1 | 135.394 (11) |
| H8A—C8—H8C | 109.5 | S2—Ni1—P1 | 44.606 (11) |
| H8B—C8—H8C | 109.5 | S1—Ni1—P1 | 44.737 (12) |
| O2—C9—H9A | 109.5 | S1^i—Ni1—P1 | 135.263 (12) |
| O2—C9—H9B | 109.5 | P1^i—Ni1—P1 | 180.0 |
| H9A—C9—H9B | 109.5 | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.8 (2) | C1—P1—S2—Ni1 | −109.65 (5) |
| P1—C1—C2—C3 | 174.69 (12) | S1—P1—S2—Ni1 | 11.639 (18) |
| C1—C2—C3—C4 | −0.5 (2) | P1—S2—Ni1—S2^i | 67 (100) |
| C2—C3—C4—O1 | −178.75 (14) | P1—S2—Ni1—S1 | −10.140 (16) |
| C2—C3—C4—C5 | 1.9 (2) | P1—S2—Ni1—S1^i | 169.860 (16) |
| O1—C4—C5—C6 | 178.78 (14) | P1—S2—Ni1—P1^i | 180.0 |
| C3—C4—C5—C6 | −1.9 (2) | P1—S1—Ni1—S2^i | −169.884 (16) |
| C2—C1—C6—C5 | 0.7 (2) | P1—S1—Ni1—S2 | 10.116 (16) |
| P1—C1—C6—C5 | −174.82 (13) | P1—S1—Ni1—S1^i | −11 (100) |
| C4—C5—C6—C1 | 0.6 (2) | P1—S1—Ni1—P1^i | 180.0 |
| C5—C4—O1—C7 | 1.5 (2) | O2—P1—Ni1—S2^i | 97.35 (7) |
| C3—C4—O1—C7 | −177.89 (13) | C1—P1—Ni1—S2^i | −81.64 (6) |
| C8—C7—O1—C4 | 178.93 (13) | S2—P1—Ni1—S2^i | 180.000 (1) |
| C9—O2—P1—C1 | −177.47 (12) | S1—P1—Ni1—S2^i | 14.48 (2) |
| C9—O2—P1—S2 | −54.64 (12) | O2—P1—Ni1—S2 | −82.65 (7) |
| C9—O2—P1—S1 | 61.90 (12) | C1—P1—Ni1—S2 | 98.36 (6) |
| C9—O2—P1—Ni1 | 3.43 (15) | S1—P1—Ni1—S2 | −165.52 (2) |
| C6—C1—P1—O2 | −74.92 (13) | O2—P1—Ni1—S1 | 82.87 (7) |
| C2—C1—P1—O2 | 109.62 (12) | C1—P1—Ni1—S1 | −96.12 (6) |
| C6—C1—P1—S2 | 162.44 (11) | S2—P1—Ni1—S1 | 165.52 (2) |
| C2—C1—P1—S2 | −13.02 (14) | O2—P1—Ni1—S1^i | −97.13 (7) |
| C6—C1—P1—S1 | 46.67 (13) | C1—P1—Ni1—S1^i | 83.88 (6) |
| C2—C1—P1—S1 | −128.78 (11) | S2—P1—Ni1—S1^i | −14.48 (2) |
| C6—C1—P1—Ni1 | 104.40 (12) | S1—P1—Ni1—S1^i | 180.0 |
| C2—C1—P1—Ni1 | −71.06 (13) | O2—P1—Ni1—P1^i | −20 (100) |
| O2—P1—S1—Ni1 | −134.48 (4) | C1—P1—Ni1—P1^i | 161 (100) |
| C1—P1—S1—Ni1 | 110.92 (5) | S2—P1—Ni1—P1^i | 63 (100) |

| S2—P1—S1—Ni1 | −11.583 (18) | S1—P1—Ni1—P1ⁱ | −102 (100) |
| O2—P1—S2—Ni1 | 134.46 (5) | | |

Symmetry code: (i) −*x*+2, −*y*+2, −*z*+2.

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
| --- | --- | --- | --- | --- |
| C3—H3···O1ⁱⁱ | 0.95 | 2.57 | 3.5123 (18) | 171 |

Symmetry code: (ii) −*x*+1, −*y*+1, −*z*+2.