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Crystal structure of chlorido{tris[2-(isopropylsulfanyl)phenyl]phosphane-κ^4P,S,S',S''}nickel(II) trifluoromethanesulfonate

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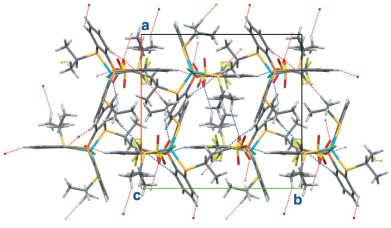
The complex cation of the title compound, $[NiCl\{P(C_6H_4\text{-}2\text{-}S\text{-}i\text{-}Pr)_3\}](CF_3SO_3)$, has a slightly distorted trigonal–bipyramidal coordination geometry in which three S atoms are located in the equatorial plane, and one P and one Cl atom in the apical positions. In the cation, there are two intramolecular C—H···S hydrogen bonds. In the crystal, there are some intermolecular C—H···O and C—H···F hydrogen bonds formed between the cation and the anion. The trifluoromethanesulfonate anion and one of the methyl groups are both disordered over two sets of sites with occupancies of 0.629 (17):0.371 (17) and 0.786 (14):0.214 (14), respectively.

1. Chemical context

Unusual five-coordinate nickel(II) complexes have been often obtained by use of polydentate ligands such as tripodal tetradentate ligands (Orioli, 1971; Morassi *et al.*, 1973; Hierso *et al.*, 2003). A variety of tripodal tetradentate ligands having phosphines and/or amines as coordinating sites have been used for the synthesis of five-coordinate nickel(II) complexes. However, for PS_3-type tripodal tetradentate ligands in which three thioether moieties are tethered to a phosphine moiety, only one crystal structure (Haugen & Eisenberg, 1969) had been reported before we started our studies. Recently, we have synthesized new PS_3-type tripodal tetradentate ligands, tris(2-isopropylthiophenyl)phosphine, **1a** and tris(2-*tert*-butylthiophenyl)phosphine, **1b** (Fig. 1), and reported the syntheses and properties of their group 10 metal complexes (Takeda *et al.*, 2010, 2016). Reaction of **1a** with $NiCl_2{\cdot}6H_2O$ in



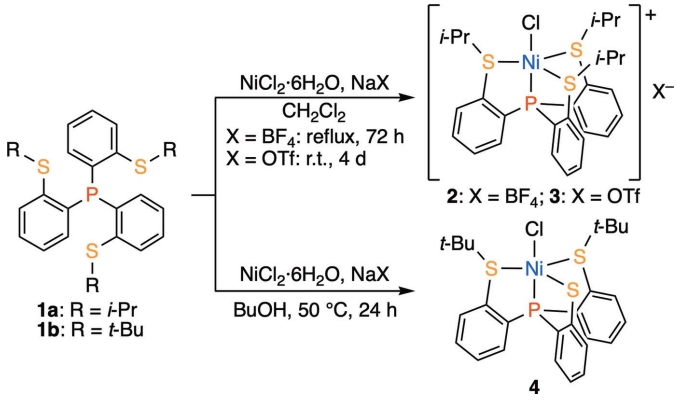
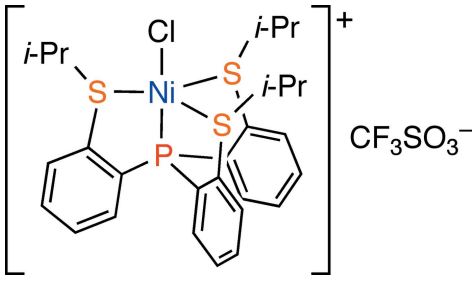


Figure 1
Synthesis of nickel(II) complexes bearing the PS_3-type tripodal tetradentate ligand.

the presence of $NaBF_4$ gave the corresponding cationic five-coordinate nickel(II) complex, **2**, while the reaction of **1b** with $NiCl_2{\cdot}6H_2O$ resulted in the elimination of *t*-BuCl to afford a neutral five-coordinate nickel(II) complex, **4** (Fig. 1). In this paper, we describe the structure of the title compound, $[NiCl(L)]CF_3SO_3$ (L = **1a**), **3**, which was prepared by reaction of **1a** with $NiCl_2{\cdot}6H_2O$ in the presence of an excess amount of $NaCF_3SO_3$ (Fig. 1).



2. Structural commentary

The structure of the title compound, **3**, is shown in Fig. 2. The triflate anion and one of the methyl groups are each disordered over two sets of sites with occupancies of 0.629 (17):0.371 (17) and 0.786 (14):0.214 (14), respectively. The complex cation of **3** has a five-coordinate slightly distorted trigonal–bipyramidal structure, in which one P atom and one Cl atom coordinate to the nickel center(II) in the apical positions [P1—Ni1—Cl1 177.83 (5)°] and three S atoms are located in the equatorial positions. In addition, there are two weak C—H···S intramolecular hydrogen bonds (C26—H26*B*···S1 and C17—H17*B*···S3; Table 1). Table 2 presents selected bond lengths and angles of **3** along with those of the related complexes, complex **2** (Takeda *et al.*, 2010) and the methyl derivative, $[NiCl\{P(C_6H_4\text{-}2\text{-}SCH_3)_3\}]ClO_4$, **5** (Haugen & Eisenberg, 1969). The conformation of the Ni(S-*i*-Pr)$_3$ unit of **3** is similar to that of complex **2**, but different from that of **5**, as shown in Fig. 3. This is probably due to the difference in the bulkiness between the isopropyl and methyl groups. In **3**, the

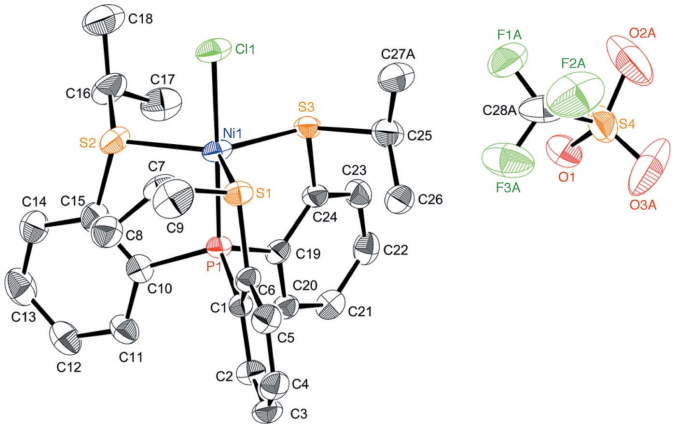


Figure 2
The molecular structure of the title compound, **3**. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms and minor disorder components are omitted for clarity.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.95	2.42	3.336 (5)	162
C5—H5···O3*B*^{ii}	0.95	2.55	3.328 (11)	140
C8—H8···F2*A*^{iii}	0.98	2.53	3.318 (14)	138
C8—H8···F2*B*^{iii}	0.98	2.50	3.30 (2)	139
C17—H17*B*···S3	0.98	2.82	3.652 (5)	143
C18—H18*B*···F3*B*^{iv}	0.98	2.15	3.099 (12)	162
C20—H20···O1^{i}	0.95	2.58	3.477 (5)	157
C22—H22···O2*A*^{v}	0.95	2.31	3.127 (12)	144
C26—H26*B*···S1	0.98	2.85	3.762 (6)	156
C27*B*—H27*D*···O1	0.98	2.46	3.308 (19)	144

Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $x+1, y, z$; (v) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

Table 2
Selected bond distances (Å) and angles (°) in complexes **2**, **3** and **5**.

compounds	**3**	**2**^{a}	**5**^{b}
Ni1—P1	2.1124 (11)	2.1108 (7)	2.113 (7)
Ni1—S1	2.2574 (12)	2.2454 (7)	2.242 (8)
Ni1—S2	2.2612 (13)	2.2678 (7)	2.269 (6)
Ni1—S3	2.3072 (13)	2.3510 (7)	2.290 (7)
Ni1—Cl	2.2412 (11)	2.2437 (7)	2.227 (7)
P1—Ni1—Cl1	177.83 (5)	178.60 (3)	178.5 (3)
S2—Ni1—S3	120.87 (5)	109.53 (3)	112.1 (3)
S3—Ni1—S1	116.04 (5)	119.03 (3)	127.1 (3)
S1—Ni1—S2	122.83 (5)	130.74 (3)	120.6 (2)
P1—Ni1—S	88.16 (4)–88.1 (4)	86.9 – 87.5	88.0 – 88.7
Cl1—Ni1—S	89.88 (4)–93.48 (5)	92.0 – 94.5	90.7 – 92.4

Notes: (*a*) Takeda *et al.* (2010); (*b*) Haugen & Eisenberg (1969).

Ni1—S3 bond length [2.3072 (13) Å] is slightly longer than the Ni1—S1 and Ni1—S2 bond lengths [2.2574 (12) and 2.2612 (13) Å, respectively], and the S1—Ni1—S2 bond angle [122.83 (5)°] is slightly larger than the S2—Ni1—S3 and S3—Ni1—S1 bond angles [120.87 (5) and 116.04 (5)°, respectively]. This properties suggests that in complex **3** the five-coordinate trigonal–bipyramidal structure slightly approaches a four-coordinate square-planar structure by the elongation of the Ni—S3 bond. This is a similar tendency to the structure of **2**, and the deviation from trigonal–bipyramidal structure in **3** is smaller than that in **2**. The Ni—S bond lengths of **3** are very close to those of methyl derivative **5**, while the S3—Ni—S1 bond angle of **5** [127.1 (3)°] is large as expected from the conformation **B** (Fig. 3).

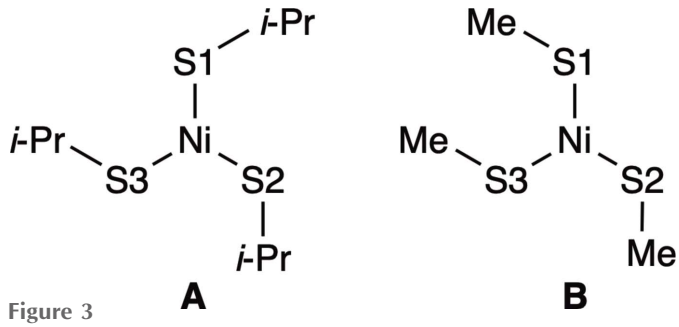


Figure 3
The conformation diagrams of the Ni(S*R*)$_3$ moieties (*R* = *i*-Pr or Me) for **3** (**A**) and **5** (**B**), viewed along the Ni—Cl bond.

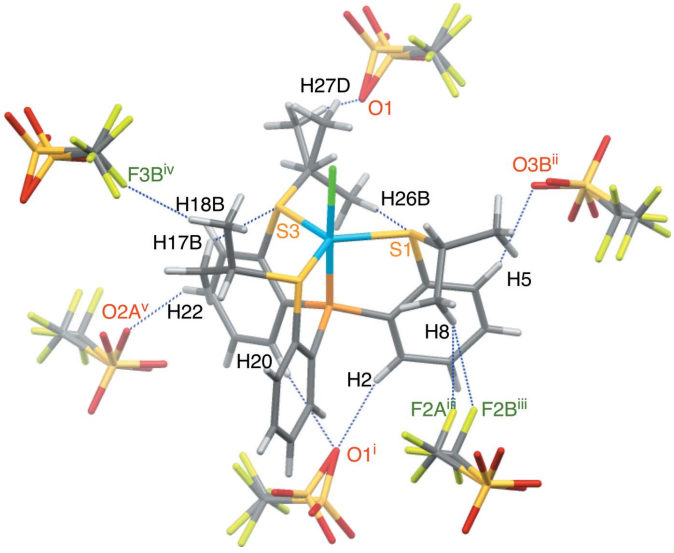


Figure 4
Intramolecular C—H···S hydrogen bonds and intermolecular C—H···O and C—H···F hydrogen bonds (blue dashed lines) in **3**. [Symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $x+1, y, z$; (v) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.]

3. Supramolecular features

In the crystal of **3**, there are some hydrogen bonds between the cation and the anion (Fig. 4). The cation and the anion are linked into a tape structure along the *b*-axis direction *via* C—H···O and C—H···F hydrogen bonds (C2—H2···O1^{i}, C8—H8···F2*A*^{iii}, C8—H8···F2*B*^{iii}, C20—H20···O1^{i} and C22—H22···O2*A*^{v}; symmetry codes as in Table 1) . The tapes are further linked by weak C—H···O and C—H···F hydrogen bonds formed between the cation and the minor component of the disordered anion (C5—H5···O3*B*^{ii} and C18—H18*B*···F3*B*^{iv}; Table 1), forming a three-dimensional network (Figs. 5 and 6).

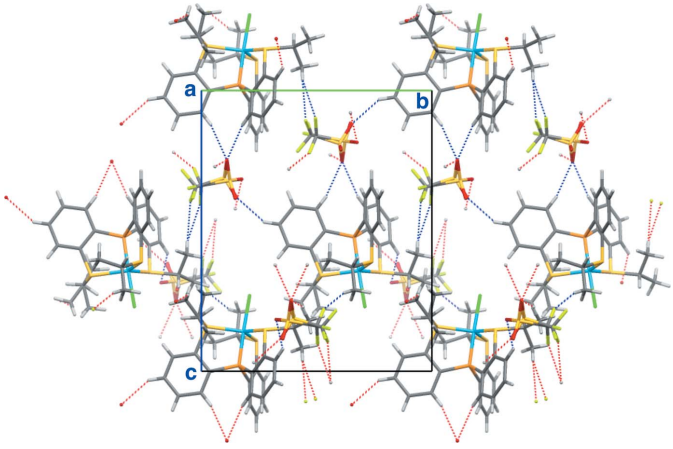


Figure 5
A packing diagram of **3**, viewed along the *a* axis. The C—H···O and C—H···F hydrogen bonds are shown as dashed lines.

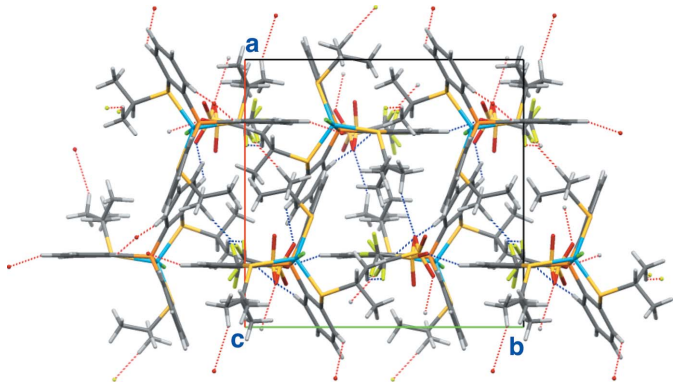


Figure 6
A packing diagram of **3**, viewed along the *c* axis. The C—H···O and C—H···F hydrogen bonds are shown as dashed lines.

4. Database survey

A search of the Cambridge Structural Database (CSD; Groom *et al.*, 2016) using WebCSD found four structures of nickel complexes having three Ni—S, one Ni—P and one Ni—Cl bonds. The structures of the complexes, [NiCl{P(C_6H_4-2-SMe)$_3$}]ClO_4, **5** (refcode: CMTPPN; Haugen & Eisenberg, 1969) and [NiCl{P(C_6H_4-2-S-*i*-Pr)$_3$}]BF_4, **2** (FULMOP; Takeda *et al.*, 2010), are similar to that of the cationic choloridonickel(II) complex **3**. The structures of the other two complexes, [Ph_3P═N═PPh_3][NiCl{P(C_6H_3-3-$SiMe_3$-2-S)$_3$}] (YETYOM; Lee *et al.*, 2006) and [NiCl{P(C_6H_4-2-S)(C_6H_4-2-S-*t*-Bu)$_2$}], **4** (EZOQAN; Takeda *et al.*, 2016), are different from that of complex **3**. The former is an anionic nickel(III) complex having three thiolato ($^{-}$*SR*), one chlorido and one phosphine ligands, and the latter, **4**, is a neutral nickel(II) complex having two thioether, one thiolato, one chlorido and one phosphine ligands.

5. Synthesis and crystallization

A mixture of tris(2-isopropylthiophenyl)phosphine, **1a** (0.141 g, 0.291 mmol), $NiCl_2{\cdot}6H_2O$ (0.060 g, 0.25 mmol) and $NaCF_3SO_3$ (0.345 g, 2.01 mmol) in dichloromethane (5 ml) was stirred at room temperature for 4 d. After removal of the solvent under reduced pressure, recrystallization of the residue from a chloroform/hexane solution gave the title compound, **3**, as blue crystals (0.168 g, 91%).

M.p. 485 K (decomp.) ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.31 (*d*, $^3J_{HH}$ = 6.7 Hz, 18H), 3.73 (*sepd*, $^3J_{HH}$ = 6.7 Hz, $^4J_{HP}$ = 1.6 Hz, 3H), 7.71 (*tdd*, $^3J_{HH}$ = 8.3 Hz, J_{HP} = 2.2 Hz, $^4J_{HH}$ = 1.0 Hz, 3H), 7.80 (*ddd*, $^3J_{HH}$ = 8.3 Hz, $^4J_{HP}$ = 3.3 Hz, $^4J_{HH}$ = 1.0 Hz, 3H), 7.91 (*tdd*, $^3J_{HH}$ = 8.3 Hz, J_{HP} = 2.5 Hz, $^4J_{HH}$ = 1.0 Hz, 3H), 8.68 (*dd*, $^3J_{HH}$ = 8.3 Hz, $^3J_{HP}$ = 8.3 Hz, 3H). ^{13}C{^{1}H} NMR (150 MHz, $CDCl_3$): δ 22.3 (*s*, CH_3), 50.7 (*s*, CH), 132.9 (*d*, J_{CP} = 7.2 Hz, CH), 133.4 (*d*, J_{CP} = 13.0 Hz, CH), 133.6 (*s*, CH), 134.8 (*s*, CH), 135.3 (*d*, $^1J_{CP}$ =63.6 Hz, C), 137.0 (*d*, $^2J_{CP}$ = 23.1 Hz, C), the peak of CF_3 could not be detected. ^{31}P NMR (162 MHz, $CDCl_3$): δ 103.3. ^{19}F NMR (376 MHz, $CDCl_3$): δ −77.92. IR (KBr): 516.9, 532.3, 551.6, 572.8, 638.4,

Table 3
Experimental details.

Crystal data	
Chemical formula	$[NiCl(C_{27}H_{33}PS_3)](CF_3SO_3)$
M_r	727.91
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	120
a, b, c (Å)	13.428 (3), 14.008 (3), 17.110 (3)
β (°)	93.164 (4)
V (Å^3)	3213.5 (11)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	1.04
Crystal size (mm)	0.10 × 0.08 × 0.02
Data collection	
Diffractometer	Rigaku CrystalClear-SM Expert 2.1 b29
Absorption correction	Numerical (*CrystalClear*; Rigaku, 2013)
T_{min}, T_{max}	0.924, 0.971
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	51723, 7359, 5054
R_{int}	0.096
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.144, 1.08
No. of reflections	7359
No. of parameters	451
No. of restraints	20
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.75, −0.35

Computer programs: *CrystalClear* (Rigaku, 2013), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *Yadokari-XG* (Wakita, 2001; Kabuto *et al.*, 2009) and *publCIF* (Westrip, 2010).

673.1, 727.1, 740.6, 779.2, 879.5, 931.6, 1029.9, 1056.9 (S═O), 1116.7, 1157.2 (S═O),1224.7, 1242.1, 1249.8, 1265.2, 1274.9, 1282.6, 1369.4, 1388.7, 1433.0, 1460.0, 1568.0, 1635.5, 2868.0, 2927.7, 2968.2, 3055.0, 3082.0, 3301.9, 3319.3, 3392.6, 3406.1, 3423.4, 3444.6, 3477.4, 3489.0. UV–vis ($CHCl_3$): λ_{max} 246 (ε 35000), 332 (ε 5700), 474 (ε 350), 639 nm (ε 2000). Analysis calculated for $C_{28}H_{33}ClF_3NiO_3PS_4$: C 46.20, H 4.57%. Found: C 45.38, H 4.55%.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The H atoms were positioned geometrically (C—H = 0.95–1.00 Å) and refined as riding atoms with U_{iso}(H) =1.5U_{eq}(C) for methyl or 1.2U_{eq}(C) for aromatic and methine H atoms. The methyl groups were allowed to rotate freely around the C—C bond. The triflate anion exhibits disorder and was modelled with occupancies of 0.629 (17) and 0.371 (17). The geometric parameters of the minor component were restrained to be similar to those of the major component by using *SAME* restraint. In addition, one of the methyl groups in the complex cation exhibits disorder and was modelled with occupancies of 0.786 (14) and 0.214 (14). The C25—C27*A* and C25—C27*B* bond lengths were restrained to be equal to each other by using *SADI* restraint.

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supporting information

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Nobuhiro Takeda, Rin Oma and Masafumi Unno

Computing details

Data collection: *CrystalClear* (Rigaku, 2013); cell refinement: *CrystalClear* (Rigaku, 2013); data reduction: *CrystalClear* (Rigaku, 2013); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015*a*); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015*b*); molecular graphics: *Yadokari-XG* (Wakita, 2001; Kabuto *et al.*, 2009); software used to prepare material for publication: *Yadokari-XG* (Wakita, 2001; Kabuto *et al.*, 2009) and *publCIF* (Westrip, 2010).

Chlorido{tris[2-(isopropylsulfanyl)phenyl]phosphane-κ^4P,S,S',S''}nickel(II) trifluoromethanesulfonate

Crystal data

$[NiCl(C_{27}H_{33}PS_3)](CF_3SO_3)$
$M_r = 727.91$
Monoclinic, $P2_1/n$
$a = 13.428$ (3) Å
$b = 14.008$ (3) Å
$c = 17.110$ (3) Å
$\beta = 93.164$ (4)°
$V = 3213.5$ (11) Å^3
$Z = 4$
$F(000) = 1504$
$D_x = 1.505$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 5728 reflections
$\theta = 2.8$–27.5°
$\mu = 1.04$ mm^{-1}
$T = 120$ K
Prism, blue
0.10 × 0.08 × 0.02 mm

Data collection

Rigaku CrystalClear-SM Expert 2.1 b29 diffractometer
Radiation source: Rotating Anode
Confocal monochromator
Detector resolution: 5.8140 pixels mm^{-1}
profile data from ω–scans
Absorption correction: numerical (CrystalClear; Rigaku, 2013)
$T_{min} = 0.924$, $T_{max} = 0.971$
51723 measured reflections
7359 independent reflections
5054 reflections with $I > 2\sigma(I)$
$R_{int} = 0.096$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.8°$
$h = -17\rightarrow17$
$k = -18\rightarrow18$
$l = -22\rightarrow22$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.057$
$wR(F^2) = 0.144$
$S = 1.08$
7359 reflections
451 parameters
20 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0517P)^2 + 5.7574P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.75$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}

Special details

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

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
Ni1	0.75663 (4)	0.31726 (4)	0.35830 (3)	0.02972 (15)	
Cl1	0.77545 (8)	0.29069 (9)	0.23080 (6)	0.0409 (3)	
P1	0.73682 (7)	0.33699 (7)	0.47886 (5)	0.0246 (2)	
C1	0.6229 (3)	0.2789 (3)	0.5066 (2)	0.0262 (8)	
C2	0.5845 (3)	0.2845 (3)	0.5811 (2)	0.0321 (9)	
H2	0.6179	0.3205	0.6216	0.039*	
C3	0.4967 (3)	0.2363 (3)	0.5944 (3)	0.0384 (10)	
H3	0.4706	0.2389	0.6448	0.046*	
C4	0.4466 (3)	0.1846 (3)	0.5360 (3)	0.0381 (10)	
H4	0.3872	0.1516	0.5468	0.046*	
C5	0.4822 (3)	0.1805 (3)	0.4619 (3)	0.0358 (10)	
H5	0.4465	0.1470	0.4210	0.043*	
C6	0.5721 (3)	0.2269 (3)	0.4482 (2)	0.0274 (8)	
S1	0.61937 (8)	0.22394 (8)	0.35266 (6)	0.0304 (2)	
C7	0.6643 (3)	0.0991 (3)	0.3441 (3)	0.0386 (10)	
H7	0.7114	0.0985	0.3008	0.046*	
C8	0.7218 (4)	0.0635 (4)	0.4164 (3)	0.0491 (12)	
H8	0.6777	0.0613	0.4601	0.074*	
H8A	0.7778	0.1066	0.4294	0.074*	
H8B	0.7473	−0.0008	0.4067	0.074*	
C9	0.5777 (4)	0.0336 (4)	0.3189 (3)	0.0570 (14)	
H9	0.6037	−0.0287	0.3038	0.085*	
H9A	0.5396	0.0620	0.2743	0.085*	
H9B	0.5342	0.0254	0.3625	0.085*	
C10	0.8429 (3)	0.2904 (3)	0.5377 (2)	0.0297 (9)	
C11	0.8506 (4)	0.2885 (3)	0.6188 (2)	0.0364 (10)	
H11	0.7951	0.3060	0.6479	0.044*	
C12	0.9387 (4)	0.2611 (4)	0.6570 (3)	0.0460 (12)	
H12	0.9448	0.2618	0.7126	0.055*	
C13	1.0190 (4)	0.2325 (4)	0.6148 (3)	0.0515 (13)	
H13	1.0798	0.2145	0.6418	0.062*	
C14	1.0113 (3)	0.2299 (4)	0.5342 (3)	0.0471 (12)	
H14	1.0653	0.2075	0.5056	0.057*	
C15	0.9229 (3)	0.2607 (3)	0.4950 (3)	0.0364 (10)	
S2	0.91100 (8)	0.26050 (9)	0.39095 (6)	0.0383 (3)	
C16	1.0134 (4)	0.3448 (4)	0.3714 (3)	0.0515 (13)	
H16	1.0729	0.3224	0.4041	0.062*	
C17	0.9930 (4)	0.4436 (4)	0.3978 (3)	0.0529 (13)	
H17	1.0532	0.4825	0.3946	0.079*	

H17A	0.9732	0.4421	0.4521	0.079*	
H17B	0.9390	0.4713	0.3643	0.079*	
C18	1.0401 (4)	0.3352 (5)	0.2900 (3)	0.0659 (16)	
H18	0.9819	0.3502	0.2550	0.099*	
H18A	1.0617	0.2696	0.2805	0.099*	
H18B	1.0945	0.3794	0.2799	0.099*	
C19	0.7307 (3)	0.4636 (3)	0.5007 (2)	0.0270 (8)	
C20	0.7291 (3)	0.5015 (3)	0.5767 (2)	0.0297 (9)	
H20	0.7287	0.4601	0.6206	0.036*	
C21	0.7283 (3)	0.5992 (3)	0.5871 (3)	0.0341 (9)	
H21	0.7258	0.6248	0.6383	0.041*	
C22	0.7312 (3)	0.6603 (3)	0.5236 (3)	0.0370 (10)	
H22	0.7312	0.7274	0.5315	0.044*	
C23	0.7340 (3)	0.6238 (3)	0.4487 (3)	0.0372 (10)	
H23	0.7375	0.6657	0.4053	0.045*	
C24	0.7317 (3)	0.5263 (3)	0.4371 (2)	0.0288 (9)	
S3	0.72947 (8)	0.47865 (8)	0.34063 (6)	0.0310 (2)	
C25	0.6003 (3)	0.5122 (5)	0.3077 (3)	0.0551 (15)	
H25A	0.5974	0.5834	0.3110	0.066*	0.786 (14)
H25B	0.5936	0.4535	0.2745	0.066*	0.214 (14)
C26	0.5214 (3)	0.4751 (4)	0.3611 (3)	0.0459 (12)	
H26	0.4550	0.4935	0.3396	0.069*	
H26A	0.5329	0.5027	0.4135	0.069*	
H26B	0.5257	0.4054	0.3645	0.069*	
C27A	0.5825 (5)	0.4890 (6)	0.2262 (3)	0.049 (2)	0.786 (14)
H27A	0.5843	0.4195	0.2195	0.074*	0.786 (14)
H27B	0.6342	0.5184	0.1959	0.074*	0.786 (14)
H27C	0.5170	0.5132	0.2076	0.074*	0.786 (14)
C27B	0.5769 (15)	0.5677 (16)	0.2455 (12)	0.040 (7)	0.214 (14)
H27D	0.5064	0.5589	0.2292	0.059*	0.214 (14)
H27E	0.6184	0.5502	0.2024	0.059*	0.214 (14)
H27F	0.5887	0.6348	0.2596	0.059*	0.214 (14)
S4A	0.2594 (6)	0.5996 (6)	0.1890 (4)	0.0617 (17)	0.629 (17)
O1	0.3353 (3)	0.6108 (2)	0.25204 (19)	0.0508 (9)	
O2A	0.2747 (16)	0.6526 (8)	0.1192 (6)	0.119 (6)	0.629 (17)
O3A	0.1589 (6)	0.6058 (12)	0.2106 (7)	0.114 (6)	0.629 (17)
C28A	0.2734 (13)	0.4774 (10)	0.1571 (6)	0.061 (6)	0.629 (17)
F1A	0.3485 (7)	0.4632 (8)	0.1181 (5)	0.070 (2)	0.629 (17)
F2A	0.1947 (10)	0.4527 (12)	0.1075 (7)	0.104 (5)	0.629 (17)
F3A	0.2727 (9)	0.4177 (5)	0.2155 (4)	0.083 (3)	0.629 (17)
S4B	0.2809 (6)	0.6234 (5)	0.1799 (4)	0.0279 (14)	0.371 (17)
O2B	0.3381 (11)	0.6469 (12)	0.1159 (7)	0.056 (4)	0.371 (17)
O3B	0.1917 (9)	0.6754 (11)	0.1844 (6)	0.055 (4)	0.371 (17)
C28B	0.2460 (16)	0.4994 (15)	0.1619 (11)	0.060 (9)	0.371 (17)
F1B	0.320 (2)	0.4458 (15)	0.152 (2)	0.160 (17)	0.371 (17)
F2B	0.1807 (14)	0.4953 (11)	0.0986 (11)	0.061 (4)	0.371 (17)
F3B	0.1961 (17)	0.4693 (15)	0.2206 (8)	0.116 (10)	0.371 (17)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0264 (3)	0.0409 (3)	0.0222 (3)	−0.0057 (2)	0.0052 (2)	−0.0053 (2)
Cl1	0.0365 (6)	0.0615 (8)	0.0254 (5)	−0.0050 (5)	0.0077 (4)	−0.0094 (5)
P1	0.0243 (5)	0.0283 (5)	0.0214 (5)	−0.0028 (4)	0.0023 (4)	−0.0017 (4)
C1	0.024 (2)	0.027 (2)	0.028 (2)	0.0007 (16)	0.0046 (15)	0.0029 (16)
C2	0.035 (2)	0.033 (2)	0.029 (2)	−0.0028 (19)	0.0064 (17)	−0.0028 (17)
C3	0.044 (3)	0.035 (2)	0.038 (2)	0.001 (2)	0.019 (2)	0.0055 (19)
C4	0.030 (2)	0.034 (2)	0.051 (3)	−0.0036 (19)	0.014 (2)	0.006 (2)
C5	0.031 (2)	0.034 (2)	0.042 (2)	−0.0056 (19)	0.0038 (18)	−0.0005 (19)
C6	0.022 (2)	0.029 (2)	0.032 (2)	−0.0018 (17)	0.0046 (16)	0.0003 (16)
S1	0.0306 (5)	0.0352 (6)	0.0255 (5)	−0.0062 (4)	0.0021 (4)	−0.0049 (4)
C7	0.045 (3)	0.035 (2)	0.038 (2)	−0.005 (2)	0.014 (2)	−0.0136 (19)
C8	0.056 (3)	0.042 (3)	0.051 (3)	0.008 (2)	0.014 (2)	0.002 (2)
C9	0.065 (4)	0.038 (3)	0.068 (4)	−0.014 (3)	0.009 (3)	−0.020 (3)
C10	0.028 (2)	0.027 (2)	0.034 (2)	−0.0057 (17)	−0.0026 (17)	−0.0012 (16)
C11	0.047 (3)	0.032 (2)	0.030 (2)	0.001 (2)	−0.0038 (19)	0.0004 (17)
C12	0.052 (3)	0.046 (3)	0.039 (3)	0.001 (2)	−0.010 (2)	0.005 (2)
C13	0.039 (3)	0.059 (3)	0.054 (3)	−0.002 (3)	−0.015 (2)	0.009 (3)
C14	0.027 (2)	0.063 (3)	0.052 (3)	0.005 (2)	0.001 (2)	0.008 (2)
C15	0.027 (2)	0.041 (3)	0.041 (2)	−0.0025 (19)	−0.0005 (18)	0.0003 (19)
S2	0.0317 (6)	0.0464 (7)	0.0379 (6)	0.0025 (5)	0.0105 (4)	−0.0053 (5)
C16	0.028 (2)	0.068 (4)	0.061 (3)	−0.005 (2)	0.018 (2)	0.002 (3)
C17	0.040 (3)	0.064 (4)	0.055 (3)	−0.022 (3)	0.007 (2)	−0.005 (3)
C18	0.057 (4)	0.091 (5)	0.052 (3)	−0.002 (3)	0.020 (3)	−0.004 (3)
C19	0.0209 (19)	0.030 (2)	0.031 (2)	−0.0013 (16)	0.0051 (15)	−0.0012 (16)
C20	0.025 (2)	0.035 (2)	0.029 (2)	−0.0009 (17)	0.0050 (16)	0.0011 (16)
C21	0.032 (2)	0.033 (2)	0.038 (2)	−0.0042 (19)	0.0028 (18)	−0.0078 (18)
C22	0.031 (2)	0.029 (2)	0.051 (3)	0.0009 (18)	0.0029 (19)	−0.0011 (19)
C23	0.036 (2)	0.031 (2)	0.044 (3)	0.0018 (19)	0.0061 (19)	0.0096 (19)
C24	0.025 (2)	0.035 (2)	0.027 (2)	−0.0007 (17)	0.0060 (16)	0.0035 (16)
S3	0.0256 (5)	0.0430 (6)	0.0247 (5)	−0.0003 (4)	0.0048 (4)	0.0063 (4)
C25	0.029 (3)	0.096 (4)	0.040 (3)	0.009 (3)	0.002 (2)	0.022 (3)
C26	0.024 (2)	0.067 (3)	0.046 (3)	0.005 (2)	0.0067 (19)	0.014 (2)
C27A	0.034 (3)	0.079 (6)	0.035 (3)	−0.003 (3)	0.000 (3)	−0.005 (3)
C27B	0.022 (11)	0.032 (14)	0.065 (16)	0.010 (9)	0.010 (10)	0.005 (11)
S4A	0.082 (4)	0.063 (3)	0.0385 (19)	0.032 (3)	−0.009 (2)	−0.001 (2)
O1	0.059 (2)	0.054 (2)	0.0383 (18)	−0.0034 (18)	−0.0051 (16)	0.0042 (15)
O2A	0.229 (17)	0.066 (6)	0.057 (6)	0.046 (10)	−0.024 (8)	0.009 (4)
O3A	0.059 (5)	0.171 (15)	0.111 (8)	0.051 (7)	−0.012 (5)	−0.075 (9)
C28A	0.078 (12)	0.074 (12)	0.033 (7)	−0.028 (10)	0.015 (7)	−0.016 (8)
F1A	0.079 (5)	0.070 (5)	0.065 (4)	0.014 (3)	0.029 (4)	−0.008 (3)
F2A	0.093 (7)	0.151 (12)	0.066 (6)	−0.020 (8)	−0.005 (5)	−0.050 (8)
F3A	0.135 (8)	0.055 (4)	0.061 (4)	−0.023 (5)	0.026 (4)	0.002 (3)
S4B	0.036 (2)	0.032 (3)	0.015 (2)	−0.0002 (19)	0.0013 (14)	0.0037 (16)
O2B	0.069 (9)	0.068 (9)	0.031 (6)	−0.027 (8)	0.007 (6)	0.018 (5)
O3B	0.051 (7)	0.065 (9)	0.046 (6)	0.024 (6)	−0.013 (5)	−0.013 (6)

C28B	0.048 (12)	0.060 (13)	0.070 (19)	0.008 (10)	−0.023 (11)	0.021 (11)
F1B	0.25 (4)	0.056 (12)	0.17 (3)	0.068 (17)	−0.03 (2)	−0.033 (16)
F2B	0.054 (7)	0.066 (9)	0.061 (7)	−0.004 (6)	−0.017 (5)	−0.025 (6)
F3B	0.153 (18)	0.106 (15)	0.086 (9)	−0.096 (15)	−0.020 (9)	0.047 (8)

Geometric parameters (Å, º)

Ni1—P1	2.1124 (11)	C17—H17A	0.9800
Ni1—Cl1	2.2412 (11)	C17—H17B	0.9800
Ni1—S1	2.2574 (12)	C18—H18	0.9800
Ni1—S2	2.2612 (13)	C18—H18A	0.9800
Ni1—S3	2.3072 (13)	C18—H18B	0.9800
P1—C19	1.815 (4)	C19—C24	1.398 (5)
P1—C1	1.819 (4)	C19—C20	1.406 (5)
P1—C10	1.820 (4)	C20—C21	1.380 (6)
C1—C6	1.385 (5)	C20—H20	0.9500
C1—C2	1.403 (5)	C21—C22	1.385 (6)
C2—C3	1.388 (6)	C21—H21	0.9500
C2—H2	0.9500	C22—C23	1.382 (6)
C3—C4	1.379 (6)	C22—H22	0.9500
C3—H3	0.9500	C23—C24	1.380 (6)
C4—C5	1.381 (6)	C23—H23	0.9500
C4—H4	0.9500	C24—S3	1.779 (4)
C5—C6	1.401 (6)	S3—C25	1.854 (5)
C5—H5	0.9500	C25—C27B	1.341 (15)
C6—S1	1.787 (4)	C25—C27A	1.440 (7)
S1—C7	1.858 (5)	C25—C26	1.528 (6)
C7—C8	1.507 (7)	C25—H25A	1.0000
C7—C9	1.524 (7)	C25—H25B	1.0000
C7—H7	1.0000	C26—H26	0.9800
C8—H8	0.9800	C26—H26A	0.9800
C8—H8A	0.9800	C26—H26B	0.9800
C8—H8B	0.9800	C27A—H27A	0.9800
C9—H9	0.9800	C27A—H27B	0.9800
C9—H9A	0.9800	C27A—H27C	0.9800
C9—H9B	0.9800	C27B—H27D	0.9800
C10—C11	1.386 (6)	C27B—H27E	0.9800
C10—C15	1.396 (6)	C27B—H27F	0.9800
C11—C12	1.375 (6)	S4A—O3A	1.421 (8)
C11—H11	0.9500	S4A—O2A	1.432 (9)
C12—C13	1.390 (7)	S4A—O1	1.450 (7)
C12—H12	0.9500	S4A—C28A	1.809 (14)
C13—C14	1.378 (7)	O1—S4B	1.410 (8)
C13—H13	0.9500	C28A—F1A	1.255 (19)
C14—C15	1.398 (6)	C28A—F3A	1.302 (13)
C14—H14	0.9500	C28A—F2A	1.364 (14)
C15—S2	1.779 (4)	S4B—O3B	1.408 (11)
S2—C16	1.857 (5)	S4B—O2B	1.410 (10)

C16—C18	1.462 (7)	S4B—C28B	1.822 (17)
C16—C17	1.487 (8)	C28B—F1B	1.26 (2)
C16—H16	1.0000	C28B—F3B	1.307 (17)
C17—H17	0.9800	C28B—F2B	1.357 (17)
P1—Ni1—Cl1	177.83 (5)	H17—C17—H17A	109.5
P1—Ni1—S1	88.34 (4)	C16—C17—H17B	109.5
Cl1—Ni1—S1	89.88 (4)	H17—C17—H17B	109.5
P1—Ni1—S2	88.16 (4)	H17A—C17—H17B	109.5
Cl1—Ni1—S2	91.78 (4)	C16—C18—H18	109.5
S1—Ni1—S2	122.83 (5)	C16—C18—H18A	109.5
P1—Ni1—S3	88.41 (4)	H18—C18—H18A	109.5
Cl1—Ni1—S3	93.48 (5)	C16—C18—H18B	109.5
S1—Ni1—S3	116.04 (5)	H18—C18—H18B	109.5
S2—Ni1—S3	120.87 (5)	H18A—C18—H18B	109.5
C19—P1—C1	109.59 (18)	C24—C19—C20	119.0 (4)
C19—P1—C10	106.25 (18)	C24—C19—P1	116.8 (3)
C1—P1—C10	109.81 (18)	C20—C19—P1	124.2 (3)
C19—P1—Ni1	109.76 (13)	C21—C20—C19	119.6 (4)
C1—P1—Ni1	110.45 (13)	C21—C20—H20	120.2
C10—P1—Ni1	110.90 (14)	C19—C20—H20	120.2
C6—C1—C2	119.5 (4)	C20—C21—C22	120.8 (4)
C6—C1—P1	115.8 (3)	C20—C21—H21	119.6
C2—C1—P1	124.7 (3)	C22—C21—H21	119.6
C3—C2—C1	118.7 (4)	C23—C22—C21	120.1 (4)
C3—C2—H2	120.7	C23—C22—H22	120.0
C1—C2—H2	120.7	C21—C22—H22	120.0
C4—C3—C2	121.4 (4)	C24—C23—C22	119.9 (4)
C4—C3—H3	119.3	C24—C23—H23	120.1
C2—C3—H3	119.3	C22—C23—H23	120.1
C3—C4—C5	120.5 (4)	C23—C24—C19	120.7 (4)
C3—C4—H4	119.7	C23—C24—S3	120.2 (3)
C5—C4—H4	119.7	C19—C24—S3	119.1 (3)
C4—C5—C6	118.6 (4)	C24—S3—C25	98.9 (2)
C4—C5—H5	120.7	C24—S3—Ni1	104.55 (14)
C6—C5—H5	120.7	C25—S3—Ni1	115.2 (2)
C1—C6—C5	121.2 (4)	C27B—C25—C26	122.1 (9)
C1—C6—S1	119.1 (3)	C27A—C25—C26	114.8 (5)
C5—C6—S1	119.7 (3)	C27B—C25—S3	124.2 (9)
C6—S1—C7	103.16 (19)	C27A—C25—S3	109.8 (4)
C6—S1—Ni1	106.14 (13)	C26—C25—S3	113.6 (3)
C7—S1—Ni1	106.29 (15)	C27A—C25—H25A	105.9
C8—C7—C9	112.4 (4)	C26—C25—H25A	105.9
C8—C7—S1	113.6 (3)	S3—C25—H25A	105.9
C9—C7—S1	110.1 (3)	C27B—C25—H25B	91.0
C8—C7—H7	106.8	C26—C25—H25B	91.0
C9—C7—H7	106.8	S3—C25—H25B	91.0
S1—C7—H7	106.8	C25—C26—H26	109.5

C7—C8—H8	109.5	C25—C26—H26A	109.5
C7—C8—H8A	109.5	H26—C26—H26A	109.5
H8—C8—H8A	109.5	C25—C26—H26B	109.5
C7—C8—H8B	109.5	H26—C26—H26B	109.5
H8—C8—H8B	109.5	H26A—C26—H26B	109.5
H8A—C8—H8B	109.5	C25—C27A—H27A	109.5
C7—C9—H9	109.5	C25—C27A—H27B	109.5
C7—C9—H9A	109.5	H27A—C27A—H27B	109.5
H9—C9—H9A	109.5	C25—C27A—H27C	109.5
C7—C9—H9B	109.5	H27A—C27A—H27C	109.5
H9—C9—H9B	109.5	H27B—C27A—H27C	109.5
H9A—C9—H9B	109.5	C25—C27B—H27D	109.5
C11—C10—C15	120.1 (4)	C25—C27B—H27E	109.5
C11—C10—P1	125.0 (3)	H27D—C27B—H27E	109.5
C15—C10—P1	114.7 (3)	C25—C27B—H27F	109.5
C12—C11—C10	119.7 (4)	H27D—C27B—H27F	109.5
C12—C11—H11	120.1	H27E—C27B—H27F	109.5
C10—C11—H11	120.1	O3A—S4A—O2A	111.6 (8)
C11—C12—C13	120.4 (4)	O3A—S4A—O1	116.0 (5)
C11—C12—H12	119.8	O2A—S4A—O1	115.9 (7)
C13—C12—H12	119.8	O3A—S4A—C28A	104.6 (8)
C14—C13—C12	120.7 (4)	O2A—S4A—C28A	102.6 (6)
C14—C13—H13	119.6	O1—S4A—C28A	104.2 (6)
C12—C13—H13	119.6	F1A—C28A—F3A	110.3 (14)
C13—C14—C15	119.1 (5)	F1A—C28A—F2A	104.3 (11)
C13—C14—H14	120.4	F3A—C28A—F2A	106.0 (10)
C15—C14—H14	120.4	F1A—C28A—S4A	114.2 (9)
C10—C15—C14	119.9 (4)	F3A—C28A—S4A	111.8 (9)
C10—C15—S2	119.7 (3)	F2A—C28A—S4A	109.7 (12)
C14—C15—S2	120.4 (3)	O3B—S4B—O1	114.7 (7)
C15—S2—C16	98.8 (2)	O3B—S4B—O2B	115.0 (9)
C15—S2—Ni1	106.11 (14)	O1—S4B—O2B	115.6 (7)
C16—S2—Ni1	114.20 (18)	O3B—S4B—C28B	106.9 (9)
C18—C16—C17	115.8 (5)	O1—S4B—C28B	98.3 (7)
C18—C16—S2	109.6 (4)	O2B—S4B—C28B	103.7 (9)
C17—C16—S2	112.7 (3)	F1B—C28B—F3B	111 (2)
C18—C16—H16	106.0	F1B—C28B—F2B	110.3 (19)
C17—C16—H16	106.0	F3B—C28B—F2B	105.3 (16)
S2—C16—H16	106.0	F1B—C28B—S4B	113.1 (17)
C16—C17—H17	109.5	F3B—C28B—S4B	108.4 (13)
C16—C17—H17A	109.5	F2B—C28B—S4B	109.0 (14)

C19—P1—C1—C6	125.3 (3)	C15—S2—C16—C17	−66.9 (4)
C10—P1—C1—C6	−118.4 (3)	Ni1—S2—C16—C17	45.3 (4)
Ni1—P1—C1—C6	4.2 (3)	C1—P1—C19—C24	−116.7 (3)
C19—P1—C1—C2	−54.1 (4)	C10—P1—C19—C24	124.7 (3)
C10—P1—C1—C2	62.3 (4)	Ni1—P1—C19—C24	4.8 (3)
Ni1—P1—C1—C2	−175.1 (3)	C1—P1—C19—C20	66.1 (4)

C6—C1—C2—C3	0.9 (6)	C10—P1—C19—C20	−52.5 (4)
P1—C1—C2—C3	−179.8 (3)	Ni1—P1—C19—C20	−172.5 (3)
C1—C2—C3—C4	−0.8 (7)	C24—C19—C20—C21	0.2 (6)
C2—C3—C4—C5	−0.8 (7)	P1—C19—C20—C21	177.5 (3)
C3—C4—C5—C6	2.4 (7)	C19—C20—C21—C22	−1.4 (6)
C2—C1—C6—C5	0.7 (6)	C20—C21—C22—C23	0.5 (7)
P1—C1—C6—C5	−178.6 (3)	C21—C22—C23—C24	1.4 (7)
C2—C1—C6—S1	177.8 (3)	C22—C23—C24—C19	−2.6 (6)
P1—C1—C6—S1	−1.6 (4)	C22—C23—C24—S3	177.1 (3)
C4—C5—C6—C1	−2.3 (6)	C20—C19—C24—C23	1.7 (6)
C4—C5—C6—S1	−179.4 (3)	P1—C19—C24—C23	−175.7 (3)
C1—C6—S1—C7	110.1 (3)	C20—C19—C24—S3	−177.9 (3)
C5—C6—S1—C7	−72.9 (4)	P1—C19—C24—S3	4.7 (4)
C1—C6—S1—Ni1	−1.5 (4)	C23—C24—S3—C25	−71.4 (4)
C5—C6—S1—Ni1	175.6 (3)	C19—C24—S3—C25	108.3 (4)
C6—S1—C7—C8	−43.9 (4)	C23—C24—S3—Ni1	169.5 (3)
Ni1—S1—C7—C8	67.5 (3)	C19—C24—S3—Ni1	−10.9 (3)
C6—S1—C7—C9	83.1 (4)	C24—S3—C25—C27B	121.1 (14)
Ni1—S1—C7—C9	−165.4 (3)	Ni1—S3—C25—C27B	−128.1 (14)
C19—P1—C10—C11	63.9 (4)	C24—S3—C25—C27A	174.4 (5)
C1—P1—C10—C11	−54.5 (4)	Ni1—S3—C25—C27A	−74.8 (5)
Ni1—P1—C10—C11	−176.9 (3)	C24—S3—C25—C26	−55.5 (5)
C19—P1—C10—C15	−112.0 (3)	Ni1—S3—C25—C26	55.3 (5)
C1—P1—C10—C15	129.6 (3)	O3A—S4A—C28A—F1A	163.6 (10)
Ni1—P1—C10—C15	7.2 (4)	O2A—S4A—C28A—F1A	47.0 (12)
C15—C10—C11—C12	2.7 (6)	O1—S4A—C28A—F1A	−74.3 (10)
P1—C10—C11—C12	−172.9 (3)	O3A—S4A—C28A—F3A	−70.4 (13)
C10—C11—C12—C13	−2.0 (7)	O2A—S4A—C28A—F3A	173.0 (12)
C11—C12—C13—C14	−0.8 (8)	O1—S4A—C28A—F3A	51.8 (13)
C12—C13—C14—C15	2.9 (8)	O3A—S4A—C28A—F2A	46.9 (11)
C11—C10—C15—C14	−0.6 (7)	O2A—S4A—C28A—F2A	−69.7 (12)
P1—C10—C15—C14	175.5 (4)	O1—S4A—C28A—F2A	169.1 (9)
C11—C10—C15—S2	178.4 (3)	O3B—S4B—C28B—F1B	176 (2)
P1—C10—C15—S2	−5.5 (5)	O1—S4B—C28B—F1B	−65 (2)
C13—C14—C15—C10	−2.2 (7)	O2B—S4B—C28B—F1B	54 (2)
C13—C14—C15—S2	178.8 (4)	O3B—S4B—C28B—F3B	−61.0 (16)
C10—C15—S2—C16	119.9 (4)	O1—S4B—C28B—F3B	58.1 (15)
C14—C15—S2—C16	−61.1 (4)	O2B—S4B—C28B—F3B	177.1 (14)
C10—C15—S2—Ni1	1.5 (4)	O3B—S4B—C28B—F2B	53.1 (16)
C14—C15—S2—Ni1	−179.5 (4)	O1—S4B—C28B—F2B	172.2 (14)
C15—S2—C16—C18	162.6 (4)	O2B—S4B—C28B—F2B	−68.9 (16)
Ni1—S2—C16—C18	−85.2 (4)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O1^{i}	0.95	2.42	3.336 (5)	162
C5—H5···O3*B*^{ii}	0.95	2.55	3.328 (11)	140

C8—H8···F2*A*^{iii}	0.98	2.53	3.318 (14)	138
C8—H8···F2*B*^{iii}	0.98	2.50	3.30 (2)	139
C17—H17*B*···S3	0.98	2.82	3.652 (5)	143
C18—H18*B*···F3*B*^{iv}	0.98	2.15	3.099 (12)	162
C20—H20···O1^{i}	0.95	2.58	3.477 (5)	157
C22—H22···O2*A*^{v}	0.95	2.31	3.127 (12)	144
C26—H26*B*···S1	0.98	2.85	3.762 (6)	156
C27*B*—H27*D*···O1	0.98	2.46	3.308 (19)	144

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+1/2, *y*−1/2, −*z*+1/2; (iii) *x*+1/2, −*y*+1/2, *z*+1/2; (iv) *x*+1, *y*, *z*; (v) *x*+1/2, −*y*+3/2, *z*+1/2.