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1,3-Bis(diphenylphosphino)propane-2κ^2P,P'-dicarbonyl-1κ^2C-chloro-2κCl-{μ-2,2′,2″-nitrilotriethanethiolato(3–)-1κ^4N,S,S',S'':2κ^2S,S'}iron(II)nickel(II) acetonitrile solvate

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.009 Å
H-atom completeness 93%
R factor = 0.052
wR factor = 0.107
Data-to-parameter ratio = 11.6

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

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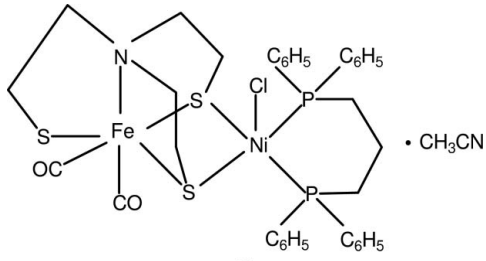
The structure of the neutral title complex, [{Fe[$(SCH_2CH_2)_3N$](CO)$_2$-S,S'}NiCl{[$P(C_6H_5)_2]_2(CH_2)_3$}]·CH_3CN or [$FeNi(C_6H_{12}NS_3)Cl(C_{27}H_{26}P_2)(CO)_2$]·$C_2H_3N$, is described. There are two independent complex molecules and two solvent molecules in the asymmetric unit. The Fe atoms are octahedrally coordinated; the three S atoms and a C atom of one of the two CO ligands form the equatorial plane, with the N atom of the $(SCH_2CH_2)_3N$ ligand and the second carbonyl C atom lying in the axial positions. The Ni atoms are square pyramidally coordinated, with the two bridging S atoms and the P atoms of the 1,3-bis(diphenylphosphino)propane ligand forming the basal plane and the Cl atom lying in the apical position.

Comment

The title compound, (I), was prepared as a further example of a synthetic structural analogue of the dimetallic active site of the enzyme nickel–iron hydrogenase (Evans & Pickett, 2003; Davies *et al.*, 1999; Smith *et al.*, 2002, 2003). Compound (I) is closely related to [{Fe[$(SCH_2CH_2)_3N$](CO)$_2$-S,S'}NiCl{[$P(C_6H_5)_2]_2(CH_2)_2$}], (II) (Davies *et al.*, 1999; Smith *et al.*, 2002), in which the chelating diphosphane is 1,2-bis(diphenylphosphino)ethane (dppe), whereas in (I) it is 1,3-bis(diphenylphosphino)propane (dppp).



(I)

The asymmetric unit consists of two complex molecules and two solvent molecules. The S_3C equatorial planes of the octahedrally coordinated Fe atoms are slightly distorted, with deviations from the mean planes lying in the range −0.069 (3) to 0.074 (3) Å in molecule 1 (the negative sign indicates the opposite side of the mean plane) and −0.060 (3) to 0.063 (3) Å in molecule 2. The Fe atoms are displaced from these mean equatorial planes by 0.067 (2) and 0.1400 (12) Å, respectively, towards the axial CO ligand. The S_2P_2 basal planes of the square pyramidally coordinated Ni atoms are also slightly distorted, with deviations from the mean planes lying in the range −0.054 (3) to 0.053 (3) Å in molecule 1 and −0.035 (3) to 0.035 (3) Å in molecule 2. The Ni atoms are displaced 0.3227 (13) and 0.3175 (14) Å, respectively, from these mean

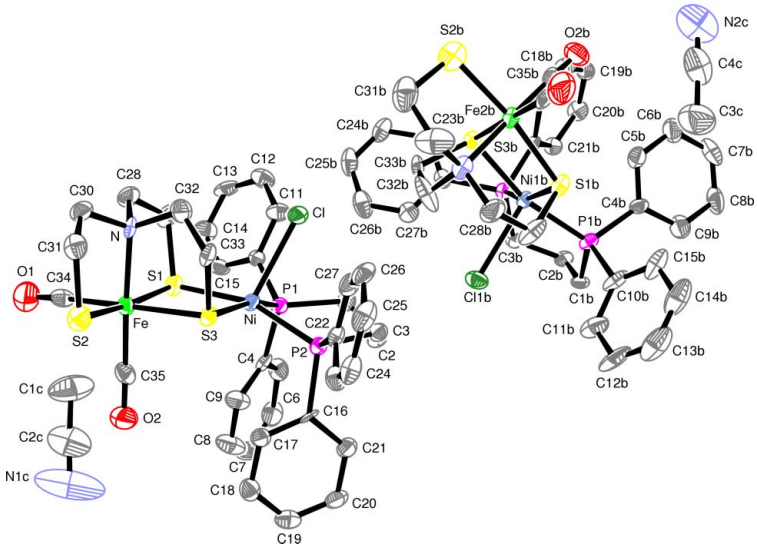


Figure 1
The asymmetric unit of (I), showing displacement ellipsoids at the 50% probability level. H atoms have been omitted.

planes, towards the Cl atoms. The S_3C and S_2P_2 mean planes are not coplanar, with an angle between their normals of 16.31 (6)°; in (II), this angle is 19.38 (7)°.

Bond dimensions about the Fe and Ni atoms are not unusual and are comparable to those in (II) [see Table 1 for dimensions in (I)]. The Fe—C bond to the equatorial CO ligand is slightly longer than those to the axial CO ligand in both molecules of (I) and in complex (II); in the second molecule of (I) it is longer than in the first and in (II) as a result of unresolved disorder in the O atom [$Fe—C_{eq}$ = 1.783 (12) Å and $Fe—C_{axial}$ = 1.741 (10) in (II)].

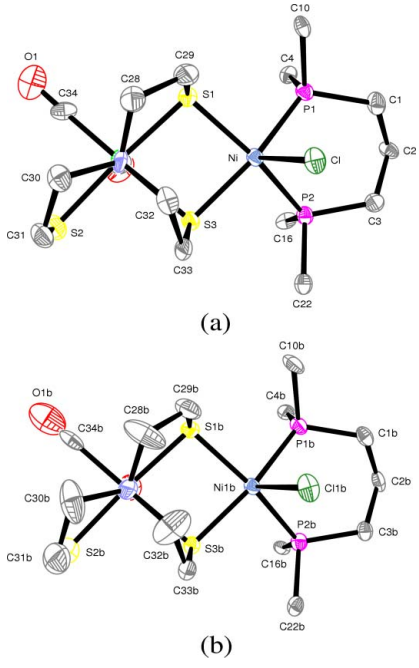


Figure 2
View along the N—Fe—C—O axis of (*a*) molecule 1 and (*b*) molecule 2, showing the deviation from the pseudo-threefold rotation of the $(SCH_2CH_2)_3N$ ligand. H atoms have been omitted.

The unusual torsion angles in the $(SCH_2CH_2)_3N$ ligand in (I) are also found in (II); the usual pseudo-threefold rotation about the Fe—N bond is removed by the non-bridging SCH_2CH_2 'arm' in both structures (see Fig. 2). Other bond dimensions in the ligands are as expected.

The molecules are arranged within the crystal structure with the complex molecules forming chains parallel to the crystallographic *a* axis; the solvent molecules occupy the centres of the channels enclosed by four such chains (see Fig. 3).

Experimental

Under an atmosphere of carbon monoxide, a mixture of $[NiCl_2(dppp)]$ (0.21 g, 0.39 mmol) and $(NEt_4)[Fe\{(SCH_2CH_2)_3N\}(CO)]$ (0.16 g, 0.39 mmol) in MeCN (100 ml) was refluxed with stirring for 2.5 h. After cooling overnight, crystals were collected by filtration and dried (0.31 g, 97%). Analysis expected for $C_{37}H_{41}ClFeN_2NiO_2P_2S_3$: C 52.1, H 4.8, N 3.3%; found C 51.7, H 4.9, N 3.2%. ν(CO), KBr: 1944 and 2006 cm^{-1}; Mössbauer (solid, 80 K, relative to iron foil at 298 K) isomer shift 0.07 mm s^{-1}, quadrupole splitting 0.56 mm s^{-1}.

Crystal data

$[FeNi(C_6H_{12}NS_3)Cl(C_{27}H_{26}P_2)(CO)_2]\cdot C_2H_3N$
M_r = 853.85
Orthorhombic, $Pca2_1$
a = 20.6025 (4) Å
b = 12.4769 (2) Å
c = 29.7090 (6) Å
V = 7636.9 (2) $Å^3$
Z = 8
D_x = 1.485 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 24708 reflections
θ = 3.7–23.8°
μ = 1.23 mm^{-1}
T = 173 (2) K
Plate, brown
0.2 × 0.2 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.823, T_{max} = 0.979
24708 measured reflections
10246 independent reflections
8837 reflections with $I > 2\sigma(I)$
R_{int} = 0.052
θ_{max} = 23.7°
$h = -22 \rightarrow 22$
$k = -14 \rightarrow 13$
$l = -27 \rightarrow 33$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.107$
$S = 1.07$
10246 reflections
884 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + 30.7123P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 0.88$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}
Absolute structure: Flack (1983), 4317 Friedel pairs
Flack parameter: 0.604 (14)

Table 1
Selected geometric parameters (Å, °).

Ni—P1	2.2012 (14)	Ni1*b*—P1*b*	2.2018 (15)
Ni—P2	2.2060 (15)	Ni1*b*—P2*b*	2.2046 (15)
Ni—S3	2.2517 (13)	Ni1*b*—S1*b*	2.2495 (16)
Ni—S1	2.2574 (15)	Ni1*b*—S3*b*	2.2536 (14)
Ni—Cl	2.5787 (14)	Ni1*b*—Cl1*b*	2.5971 (16)
Fe—C35	1.759 (6)	Fe2*b*—C35*b*	1.760 (6)
Fe—C34	1.829 (6)	Fe2*b*—C34*b*	1.912 (7)
Fe—N	2.048 (4)	Fe2*b*—N1*b*	2.065 (5)
Fe—S1	2.2865 (15)	Fe2*b*—S2*b*	2.2839 (19)
Fe—S2	2.2978 (16)	Fe2*b*—S1*b*	2.2909 (16)
Fe—S3	2.3159 (15)	Fe2*b*—S3*b*	2.3029 (15)
O1—C34	1.065 (7)	O1*b*—C34*b*	0.861 (8)
O2—C35	1.151 (7)	O2*b*—C35*b*	1.137 (7)
P1—Ni—P2	92.88 (5)	O2—C35—Fe	176.9 (5)
P1—Ni—S3	165.43 (6)	P1*b*—Ni1*b*—P2*b*	92.84 (6)
P2—Ni—S3	88.90 (5)	P1*b*—Ni1*b*—S1*b*	87.92 (6)
P1—Ni—S1	87.87 (5)	P2*b*—Ni1*b*—S1*b*	161.55 (6)
P2—Ni—S1	160.38 (6)	P1*b*—Ni1*b*—S3*b*	164.85 (6)
S3—Ni—S1	85.67 (5)	P2*b*—Ni1*b*—S3*b*	88.78 (5)
P1—Ni—Cl	88.51 (5)	S1*b*—Ni1*b*—S3*b*	85.85 (5)
P2—Ni—Cl	92.94 (5)	P1*b*—Ni1*b*—Cl1*b*	88.79 (5)
S3—Ni—Cl	105.85 (5)	P2*b*—Ni1*b*—Cl1*b*	92.29 (5)
S1—Ni—Cl	106.68 (5)	S1*b*—Ni1*b*—Cl1*b*	106.16 (6)
C35—Fe—C34	91.6 (2)	S3*b*—Ni1*b*—Cl1*b*	106.21 (5)
C35—Fe—N	175.2 (2)	C35*b*—Fe2*b*—C34*b*	90.1 (3)
C34—Fe—N	92.5 (2)	C35*b*—Fe2*b*—N1*b*	177.9 (2)
C35—Fe—S1	95.72 (19)	C34*b*—Fe2*b*—N1*b*	91.8 (2)
C34—Fe—S1	96.10 (18)	C35*b*—Fe2*b*—S2*b*	94.41 (19)
N—Fe—S1	86.26 (12)	C34*b*—Fe2*b*—S2*b*	87.86 (18)
C35—Fe—S2	90.91 (19)	N1*b*—Fe2*b*—S2*b*	86.57 (13)
C34—Fe—S2	87.63 (18)	C35*b*—Fe2*b*—S1*b*	92.44 (18)
N—Fe—S2	86.83 (12)	C34*b*—Fe2*b*—S1*b*	95.97 (18)
S1—Fe—S2	172.29 (7)	N1*b*—Fe2*b*—S1*b*	86.47 (13)
C35—Fe—S3	88.34 (18)	S2*b*—Fe2*b*—S1*b*	172.15 (7)
C34—Fe—S3	179.60 (19)	C35*b*—Fe2*b*—S3*b*	90.78 (19)
N—Fe—S3	87.58 (12)	C34*b*—Fe2*b*—S3*b*	179.1 (2)
S1—Fe—S3	83.53 (5)	N1*b*—Fe2*b*—S3*b*	87.29 (13)
S2—Fe—S3	92.76 (6)	S2*b*—Fe2*b*—S3*b*	92.30 (6)
Ni—S1—Fe	95.51 (6)	S1*b*—Fe2*b*—S3*b*	83.76 (5)
O1—C34—Fe	175.3 (5)	Ni1*B*—S1*B*—Fe2*B*	95.18 (6)
Fe—S1—C29—C28	−9.4 (6)	C29*b*—C28*b*—N1*b*—Fe2*b*	−43.0 (10)
S1—C29—C28—N	38.6 (8)	Fe2*b*—S2*b*—C31*b*—C30*b*	25.8 (8)
C29—C28—N—Fe	−51.9 (7)	S2*b*—C31*b*—C30*b*—N1*b*	−54.9 (10)
Fe—S2—C31—C30	23.7 (6)	C31*b*—C30*b*—N1*b*—Fe2*b*	58.7 (9)
S2—C31—C30—N	−51.7 (8)	Fe2*b*—S3*b*—C33*b*—C32*b*	−35.8 (7)
C31—C30—N—Fe	55.3 (7)	S3*b*—C33*b*—C32*b*—N1*b*	42.1 (10)
Fe—S3—C33—C32	−38.3 (6)	C33*b*—C32*b*—N1*b*—Fe2*b*	−24.5 (10)
S3—C33—C32—N	45.8 (8)	P1—C1—C2—C3	−68.5 (8)
C33—C32—N—Fe	−27.3 (8)	C1—C2—C3—P2	69.7 (8)
Fe2*b*—S1*b*—C29*b*—C28*b*	−3.0 (8)	P1*b*—C1*b*—C2*b*—C3*b*	−69.3 (8)
S1*b*—C29*b*—C28*b*—N1*b*	29.6 (12)	C1*b*—C2*b*—C3*b*—P2*b*	67.1 (8)

H atoms were not located for the CH_3CN solvent molecules. The value of the Flack (1983) parameter indicates an inversion twin. All other H atoms were positioned geometrically (C—H = 0.95–0.99 Å) and refined as riding [U_{iso}(H) = 1.2U_{eq}(C)].

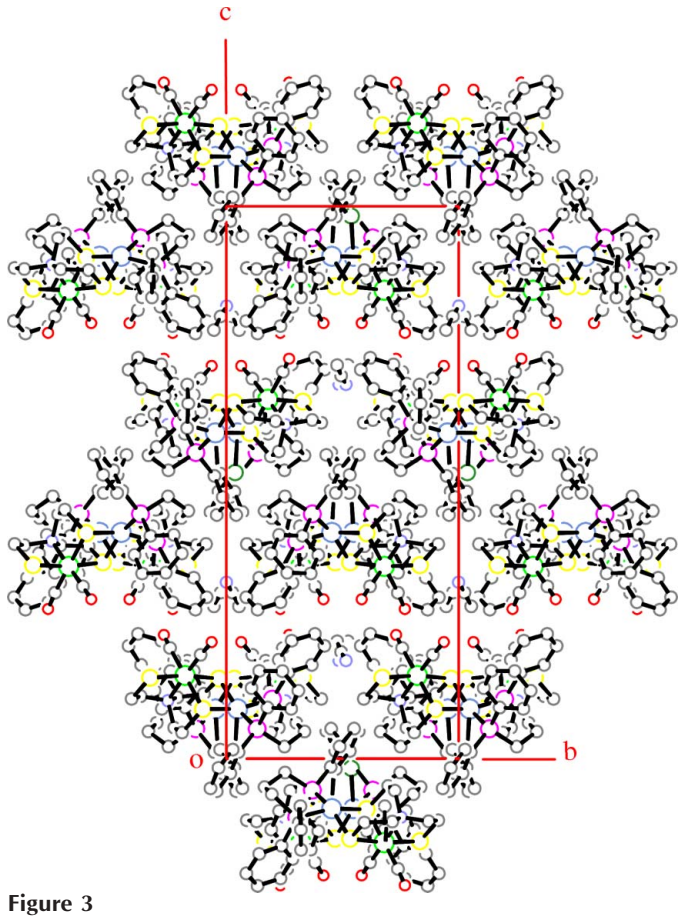


Figure 3
The packing, viewed along the crystallographic *a* axis. Atoms are represented by arbitrary spheres. H atoms have been omitted.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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supporting information

Acta Cryst. (2005). E**61**, m1316–m1319 [https://doi.org/10.1107/S1600536805018088]

1,3-Bis(diphenylphosphino)propane-2κ^2P,P'-dicarbonyl-1κ^2C-chloro-2κCl-{μ-2,2′,2″-nitrilotriethanethiolato(3–)-1κ^4N,S,S',S'':2κ^2S,S'}iron(II)nickel(II) acetonitrile solvate

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(I)

Crystal data

$[Fe(C_6H_{12}NS_3)(CO)_2NiCl(C_{27}H_{26}P_2)]\cdot C_2H_3N$
$M_r = 853.85$
Orthorhombic, $Pca2_1$
Hall symbol: P 2c -2ac
$a = 20.6025$ (4) Å
$b = 12.4769$ (2) Å
$c = 29.7090$ (6) Å
$V = 7636.9$ (2) Å^3
$Z = 8$
$F(000) = 3536$
$D_x = 1.485$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 117428 reflections
$\theta = 3.7$–$23.8°$
$\mu = 1.23$ mm^{-1}
$T = 173$ K
Plate, brown
0.2 × 0.2 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
Radiation source: Enraf–Nonius FR590
Graphite monochromator
Detector resolution: 9 pixels mm^{-1}
φ or ω? scans
Absorption correction: multi-scan (Blessing, 1995)
$T_{min} = 0.823$, $T_{max} = 0.979$
24708 measured reflections
10246 independent reflections
8837 reflections with $I > 2\sigma(I)$
$R_{int} = 0.052$
$\theta_{max} = 23.7°$, $\theta_{min} = 3.8°$
$h = -22\rightarrow22$
$k = -14\rightarrow13$
$l = -27\rightarrow33$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.107$
$S = 1.07$
10246 reflections
884 parameters
1 restraint
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
$w = 1/[\sigma^2(F_o^2) + 30.7123P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.006$
$\Delta\rho_{max} = 0.88$ e Å^{-3}
$\Delta\rho_{min} = -0.63$ e Å^{-3}
Absolute structure: Flack (1983), 4317 Friedel pairs?
Absolute structure parameter: 0.604 (14)

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. H atoms were omitted for the CH3CN solvate molecules.
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}
Ni	0.31580 (3)	0.45332 (5)	−0.09044 (2)	0.01991 (16)
Fe	0.31008 (4)	0.67952 (5)	−0.15192 (2)	0.02202 (19)
Cl	0.38331 (6)	0.46280 (10)	−0.01746 (4)	0.0283 (3)
S1	0.37554 (7)	0.53252 (10)	−0.14477 (5)	0.0261 (4)
S2	0.24863 (7)	0.83311 (11)	−0.14947 (6)	0.0371 (4)
S3	0.25547 (6)	0.60378 (9)	−0.09167 (5)	0.0222 (3)
P1	0.36558 (6)	0.30219 (10)	−0.10683 (5)	0.0213 (3)
P2	0.23460 (7)	0.37016 (10)	−0.05694 (5)	0.0206 (3)
O1	0.3765 (2)	0.7682 (4)	−0.22910 (16)	0.0607 (15)
O2	0.2146 (2)	0.5822 (4)	−0.21136 (14)	0.0522 (13)
N	0.3700 (2)	0.7517 (3)	−0.10603 (14)	0.0237 (12)
C1	0.3604 (3)	0.1952 (4)	−0.06428 (18)	0.0283 (15)
H1A	0.383	0.131	−0.0759	0.034*
H1B	0.3837	0.219	−0.0369	0.034*
C2	0.2923 (2)	0.1643 (4)	−0.05141 (18)	0.0221 (13)
H2A	0.2939	0.0985	−0.0328	0.027*
H2B	0.2676	0.1475	−0.0791	0.027*
C3	0.2562 (3)	0.2519 (4)	−0.02522 (18)	0.0247 (14)
H3A	0.2837	0.2741	0.0005	0.03*
H3B	0.216	0.2204	−0.0127	0.03*
C4	0.3346 (2)	0.2377 (4)	−0.15762 (18)	0.0233 (14)
C5	0.3599 (3)	0.1412 (4)	−0.17244 (19)	0.0338 (16)
H5	0.3976	0.1126	−0.1585	0.041*
C6	0.3306 (3)	0.0856 (5)	−0.2077 (2)	0.0453 (19)
H6	0.3457	0.0166	−0.2163	0.054*
C7	0.2780 (3)	0.1339 (6)	−0.2302 (2)	0.0494 (19)
H7	0.2583	0.0982	−0.2549	0.059*
C8	0.2550 (3)	0.2326 (6)	−0.2168 (2)	0.047 (2)
H8	0.2193	0.2644	−0.232	0.057*
C9	0.2838 (3)	0.2843 (5)	−0.18156 (18)	0.0355 (17)
H9	0.2688	0.3535	−0.1732	0.043*
C10	0.4536 (2)	0.3113 (4)	−0.11620 (17)	0.0209 (13)
C11	0.4951 (3)	0.3159 (4)	−0.0793 (2)	0.0334 (16)
H11	0.478	0.3175	−0.0496	0.04*

C12	0.5619 (3)	0.3182 (4)	−0.0861 (2)	0.0355 (16)
H12	0.5902	0.3182	−0.0609	0.043*
C13	0.5875 (3)	0.3203 (4)	−0.1287 (2)	0.0394 (17)
H13	0.6332	0.3213	−0.1329	0.047*
C14	0.5468 (3)	0.3209 (5)	−0.1650 (2)	0.0428 (18)
H14	0.5643	0.3251	−0.1946	0.051*
C15	0.4797 (3)	0.3155 (4)	−0.15904 (19)	0.0319 (16)
H15	0.4518	0.3148	−0.1845	0.038*
C16	0.1716 (2)	0.3275 (4)	−0.09666 (17)	0.0214 (13)
C17	0.1544 (3)	0.3955 (4)	−0.13105 (18)	0.0272 (15)
H17	0.1719	0.4659	−0.1318	0.033*
C18	0.1117 (3)	0.3632 (5)	−0.16473 (19)	0.0321 (16)
H18	0.1003	0.4109	−0.1884	0.039*
C19	0.0864 (3)	0.2615 (5)	−0.1633 (2)	0.0371 (17)
H19	0.0582	0.2382	−0.1866	0.045*
C20	0.1014 (3)	0.1927 (5)	−0.12845 (19)	0.0340 (16)
H20	0.0829	0.1231	−0.1273	0.041*
C21	0.1441 (3)	0.2265 (4)	−0.0948 (2)	0.0303 (15)
H21	0.1544	0.1799	−0.0705	0.036*
C22	0.1909 (3)	0.4486 (4)	−0.01484 (18)	0.0252 (14)
C23	0.1256 (3)	0.4710 (4)	−0.01890 (19)	0.0320 (15)
H23	0.1022	0.4454	−0.0443	0.038*
C24	0.0935 (3)	0.5310 (4)	0.0139 (2)	0.0384 (17)
H24	0.0483	0.5449	0.0112	0.046*
C25	0.1277 (3)	0.5698 (4)	0.0500 (2)	0.0411 (17)
H25	0.106	0.6114	0.0722	0.049*
C26	0.1925 (3)	0.5492 (4)	0.0544 (2)	0.0360 (16)
H26	0.2158	0.5771	0.0794	0.043*
C27	0.2246 (3)	0.4872 (4)	0.02205 (19)	0.0317 (16)
H27	0.2694	0.4716	0.0254	0.038*
C28	0.4397 (3)	0.7145 (4)	−0.1139 (2)	0.0360 (17)
H28A	0.4557	0.7448	−0.1426	0.043*
H28B	0.4677	0.7422	−0.0894	0.043*
C29	0.4449 (3)	0.5936 (4)	−0.1155 (2)	0.0355 (17)
H29A	0.4471	0.5653	−0.0844	0.043*
H29B	0.4855	0.5733	−0.1311	0.043*
C30	0.3694 (3)	0.8705 (4)	−0.1134 (2)	0.0317 (16)
H30A	0.3886	0.8875	−0.143	0.038*
H30B	0.3957	0.9062	−0.0899	0.038*
C31	0.2998 (3)	0.9119 (4)	−0.1115 (2)	0.0341 (16)
H31A	0.2987	0.9883	−0.1205	0.041*
H31B	0.2831	0.9063	−0.0803	0.041*
C32	0.3548 (3)	0.7250 (4)	−0.0577 (2)	0.0348 (16)
H32A	0.3664	0.7873	−0.0386	0.042*
H32B	0.3823	0.664	−0.0482	0.042*
C33	0.2844 (3)	0.6965 (4)	−0.04927 (19)	0.0273 (15)
H33A	0.2577	0.7625	−0.0499	0.033*
H33B	0.28	0.6636	−0.0191	0.033*

C34	0.3534 (3)	0.7384 (4)	−0.19960 (18)	0.0273 (15)
C35	0.2534 (3)	0.6183 (5)	−0.18797 (18)	0.0310 (16)
Ni1B	0.44894 (3)	−0.04767 (5)	0.08998 (2)	0.02046 (17)
Fe2B	0.45935 (4)	0.17831 (6)	0.15060 (3)	0.0243 (2)
Cl1B	0.37760 (7)	−0.03749 (11)	0.01804 (5)	0.0343 (4)
S1B	0.39179 (7)	0.03313 (11)	0.14485 (5)	0.0295 (4)
S2B	0.52230 (9)	0.32868 (14)	0.14654 (7)	0.0539 (5)
S3B	0.51087 (6)	0.10121 (10)	0.08990 (5)	0.0217 (3)
P1B	0.39939 (7)	−0.19807 (11)	0.10794 (5)	0.0240 (4)
P2B	0.52737 (7)	−0.13218 (10)	0.05408 (5)	0.0214 (4)
O1B	0.3979 (3)	0.2697 (4)	0.2241 (2)	0.0724 (18)
O2B	0.5449 (2)	0.0636 (3)	0.21111 (14)	0.0466 (13)
N1B	0.3986 (2)	0.2527 (3)	0.10496 (15)	0.0293 (13)
C1B	0.3990 (3)	−0.3008 (4)	0.06485 (18)	0.0254 (14)
H1B1	0.3757	−0.3643	0.0766	0.03*
H1B2	0.3745	−0.2738	0.0385	0.03*
C2B	0.4664 (3)	−0.3360 (4)	0.04915 (19)	0.0280 (15)
H2B1	0.4618	−0.401	0.0303	0.034*
H2B2	0.4925	−0.3557	0.0759	0.034*
C3B	0.5039 (3)	−0.2500 (4)	0.02196 (18)	0.0226 (14)
H3B1	0.4766	−0.2268	−0.0036	0.027*
H3B2	0.5436	−0.2833	0.0093	0.027*
C4B	0.4336 (2)	−0.2665 (4)	0.15613 (18)	0.0256 (14)
C5B	0.4853 (3)	−0.2249 (5)	0.1791 (2)	0.0340 (16)
H5B	0.5007	−0.1556	0.1712	0.041*
C6B	0.5159 (3)	−0.2807 (5)	0.2136 (2)	0.0464 (19)
H6B	0.5518	−0.2496	0.2288	0.056*
C7B	0.4944 (4)	−0.3808 (5)	0.2258 (2)	0.048 (2)
H7B	0.5161	−0.4209	0.2484	0.058*
C8B	0.4400 (4)	−0.4215 (5)	0.2042 (2)	0.049 (2)
H8B	0.4224	−0.4883	0.2137	0.059*
C9B	0.4115 (3)	−0.3675 (5)	0.1698 (2)	0.0413 (18)
H9B	0.3756	−0.3989	0.1547	0.05*
C10B	0.3133 (3)	−0.1854 (4)	0.1226 (2)	0.0365 (18)
C11B	0.2664 (3)	−0.1792 (5)	0.0880 (3)	0.0470 (19)
H11B	0.2796	−0.1817	0.0574	0.056*
C12B	0.2013 (3)	−0.1696 (5)	0.0986 (3)	0.060 (2)
H12B	0.1695	−0.1667	0.0754	0.072*
C13B	0.1832 (4)	−0.1644 (5)	0.1428 (3)	0.070 (3)
H13B	0.1384	−0.1575	0.1498	0.084*
C14B	0.2272 (3)	−0.1688 (5)	0.1773 (3)	0.064 (2)
H14B	0.2128	−0.1658	0.2077	0.076*
C15B	0.2949 (3)	−0.1780 (5)	0.1674 (2)	0.049 (2)
H15B	0.3264	−0.1791	0.1908	0.059*
C16B	0.5912 (2)	−0.1767 (4)	0.09261 (17)	0.0213 (13)
C17B	0.6102 (3)	−0.1082 (4)	0.12771 (18)	0.0266 (15)
H17B	0.5926	−0.0379	0.1294	0.032*
C18B	0.6529 (3)	−0.1410 (4)	0.1590 (2)	0.0328 (16)

H18B	0.6654	−0.0928	0.1822	0.039*
C19B	0.6788 (3)	−0.2411 (5)	0.1584 (2)	0.0325 (16)
H19B	0.7071	−0.264	0.1817	0.039*
C20B	0.6634 (3)	−0.3097 (4)	0.1230 (2)	0.0334 (16)
H20B	0.6831	−0.3784	0.1213	0.04*
C21B	0.6193 (3)	−0.2783 (4)	0.0903 (2)	0.0262 (14)
H21B	0.6084	−0.3256	0.0664	0.031*
C22B	0.5708 (3)	−0.0520 (4)	0.01205 (18)	0.0240 (14)
C23B	0.6360 (3)	−0.0269 (4)	0.0164 (2)	0.0328 (16)
H23B	0.6597	−0.0514	0.0418	0.039*
C24B	0.6667 (3)	0.0341 (5)	−0.0165 (2)	0.0386 (17)
H24B	0.7112	0.052	−0.0128	0.046*
C25B	0.6347 (3)	0.0686 (5)	−0.0536 (2)	0.0416 (18)
H25B	0.6565	0.1102	−0.0758	0.05*
C26B	0.5692 (3)	0.0419 (5)	−0.0588 (2)	0.0451 (19)
H26B	0.5464	0.0644	−0.085	0.054*
C27B	0.5377 (3)	−0.0163 (4)	−0.0265 (2)	0.0305 (16)
H27B	0.4929	−0.0327	−0.0301	0.037*
C28B	0.3314 (3)	0.2115 (6)	0.1110 (3)	0.064 (2)
H28C	0.3121	0.2485	0.1373	0.077*
H28D	0.3058	0.2328	0.0842	0.077*
C29B	0.3230 (3)	0.0976 (4)	0.1174 (3)	0.045 (2)
H29C	0.316	0.0634	0.0878	0.054*
H29D	0.2836	0.0854	0.1358	0.054*
C30B	0.3981 (4)	0.3690 (5)	0.1132 (3)	0.069 (3)
H30C	0.3817	0.3846	0.1438	0.082*
H30D	0.3699	0.4057	0.0911	0.082*
C31B	0.4712 (4)	0.4084 (5)	0.1082 (3)	0.064 (2)
H31C	0.4744	0.4854	0.1159	0.076*
H31D	0.4859	0.3988	0.0767	0.076*
C32B	0.4138 (4)	0.2251 (6)	0.0561 (2)	0.064 (2)
H32C	0.3842	0.1671	0.0464	0.077*
H32D	0.4044	0.2887	0.0373	0.077*
C33B	0.4806 (3)	0.1911 (4)	0.04729 (18)	0.0264 (15)
H33C	0.5089	0.2551	0.0459	0.032*
H33D	0.4825	0.155	0.0176	0.032*
C34B	0.4154 (3)	0.2430 (5)	0.2004 (2)	0.0323 (17)
C35B	0.5116 (3)	0.1112 (4)	0.18801 (19)	0.0305 (16)
N2	0.2291 (4)	0.4853 (8)	−0.3224 (3)	0.160 (3)
N2B	0.4973 (3)	0.0005 (6)	0.3194 (3)	0.093 (3)
C36	0.3436 (4)	0.5235 (8)	−0.2875 (3)	0.095 (3)
C37	0.2791 (5)	0.5062 (6)	−0.3067 (3)	0.081 (3)
C36B	0.3942 (4)	−0.0543 (9)	0.2759 (3)	0.099 (4)
C37B	0.4515 (4)	−0.0249 (7)	0.3007 (3)	0.068 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni	0.0181 (3)	0.0166 (3)	0.0250 (4)	−0.0006 (3)	−0.0001 (3)	0.0011 (3)
Fe	0.0248 (4)	0.0188 (4)	0.0225 (4)	0.0003 (3)	−0.0007 (3)	0.0024 (3)
Cl	0.0309 (7)	0.0225 (6)	0.0316 (8)	−0.0039 (6)	−0.0071 (6)	0.0006 (6)
S1	0.0283 (7)	0.0219 (7)	0.0282 (8)	0.0009 (6)	0.0052 (6)	0.0025 (6)
S2	0.0346 (8)	0.0296 (7)	0.0470 (9)	0.0042 (7)	−0.0003 (7)	0.0026 (7)
S3	0.0213 (6)	0.0170 (6)	0.0283 (8)	0.0006 (6)	0.0024 (6)	0.0012 (6)
P1	0.0171 (7)	0.0217 (7)	0.0250 (8)	0.0010 (6)	−0.0021 (6)	0.0013 (6)
P2	0.0231 (7)	0.0165 (6)	0.0222 (8)	−0.0011 (6)	−0.0006 (6)	0.0002 (6)
O1	0.072 (3)	0.057 (3)	0.054 (3)	−0.011 (3)	−0.001 (3)	0.008 (2)
O2	0.049 (3)	0.068 (3)	0.039 (3)	−0.015 (2)	−0.008 (2)	0.002 (2)
N	0.031 (3)	0.015 (2)	0.025 (3)	−0.003 (2)	0.0064 (19)	0.0075 (18)
C1	0.040 (3)	0.014 (3)	0.030 (3)	0.000 (3)	−0.002 (3)	−0.001 (2)
C2	0.020 (3)	0.015 (2)	0.032 (3)	0.001 (2)	0.000 (2)	−0.004 (2)
C3	0.022 (3)	0.025 (3)	0.027 (3)	−0.002 (2)	0.001 (2)	0.001 (2)
C4	0.021 (3)	0.016 (3)	0.033 (3)	−0.007 (2)	0.005 (2)	0.002 (2)
C5	0.043 (4)	0.021 (3)	0.037 (4)	0.007 (3)	−0.002 (3)	0.001 (3)
C6	0.069 (4)	0.037 (3)	0.030 (4)	−0.014 (3)	0.007 (3)	−0.007 (3)
C7	0.045 (4)	0.078 (5)	0.024 (4)	−0.024 (4)	−0.001 (3)	−0.016 (3)
C8	0.027 (3)	0.085 (5)	0.030 (4)	0.007 (4)	−0.004 (3)	−0.009 (3)
C9	0.025 (3)	0.056 (4)	0.026 (3)	0.001 (3)	0.001 (3)	−0.007 (3)
C10	0.027 (3)	0.011 (2)	0.025 (3)	0.001 (2)	−0.006 (2)	−0.001 (2)
C11	0.023 (3)	0.038 (3)	0.039 (4)	0.001 (3)	−0.004 (3)	−0.004 (3)
C12	0.034 (3)	0.037 (3)	0.036 (3)	0.009 (3)	−0.010 (3)	−0.004 (3)
C13	0.018 (3)	0.033 (3)	0.067 (4)	−0.004 (3)	−0.013 (3)	−0.003 (3)
C14	0.030 (3)	0.055 (4)	0.043 (4)	−0.001 (3)	0.006 (3)	−0.003 (3)
C15	0.023 (3)	0.043 (3)	0.030 (3)	−0.001 (3)	−0.009 (2)	0.002 (3)
C16	0.013 (2)	0.024 (3)	0.028 (3)	−0.014 (2)	0.003 (2)	−0.006 (2)
C17	0.026 (3)	0.025 (3)	0.031 (3)	−0.002 (3)	−0.004 (2)	0.001 (2)
C18	0.029 (3)	0.038 (3)	0.029 (3)	0.003 (3)	0.003 (3)	0.004 (3)
C19	0.024 (3)	0.046 (4)	0.041 (4)	0.000 (3)	−0.006 (3)	−0.005 (3)
C20	0.027 (3)	0.039 (3)	0.036 (3)	−0.013 (3)	0.000 (3)	−0.005 (3)
C21	0.027 (3)	0.027 (3)	0.037 (3)	−0.003 (2)	−0.002 (3)	0.004 (3)
C22	0.029 (3)	0.015 (3)	0.031 (3)	−0.005 (2)	0.003 (3)	0.003 (2)
C23	0.041 (3)	0.028 (3)	0.027 (3)	0.002 (3)	0.003 (3)	0.000 (3)
C24	0.041 (3)	0.032 (3)	0.042 (4)	−0.003 (3)	0.015 (3)	0.005 (3)
C25	0.049 (4)	0.031 (3)	0.044 (4)	−0.004 (3)	0.023 (3)	−0.006 (3)
C26	0.046 (4)	0.030 (3)	0.032 (3)	−0.019 (3)	0.008 (3)	−0.011 (3)
C27	0.028 (3)	0.038 (3)	0.029 (3)	−0.007 (3)	0.012 (3)	0.000 (3)
C28	0.019 (3)	0.039 (3)	0.049 (4)	−0.006 (3)	−0.003 (3)	0.009 (3)
C29	0.022 (3)	0.033 (3)	0.051 (4)	−0.003 (3)	0.007 (3)	0.005 (3)
C30	0.033 (3)	0.024 (3)	0.039 (4)	−0.006 (3)	−0.004 (3)	−0.003 (3)
C31	0.043 (4)	0.022 (3)	0.037 (4)	0.007 (3)	0.002 (3)	−0.002 (3)
C32	0.038 (3)	0.028 (3)	0.039 (4)	0.003 (3)	−0.006 (3)	0.005 (3)
C33	0.027 (3)	0.020 (3)	0.035 (3)	−0.003 (2)	0.006 (3)	0.009 (2)
C34	0.025 (3)	0.039 (3)	0.018 (3)	0.000 (3)	0.001 (2)	−0.012 (2)

C35	0.036 (3)	0.039 (3)	0.019 (3)	0.002 (3)	0.001 (3)	0.003 (3)
Ni1B	0.0192 (3)	0.0153 (3)	0.0269 (4)	0.0002 (3)	0.0012 (3)	0.0002 (3)
Fe2B	0.0289 (4)	0.0196 (4)	0.0245 (4)	−0.0009 (4)	0.0069 (3)	0.0001 (3)
Cl1B	0.0354 (8)	0.0289 (7)	0.0385 (8)	0.0039 (7)	−0.0149 (6)	−0.0001 (7)
S1B	0.0301 (8)	0.0210 (7)	0.0374 (9)	−0.0033 (6)	0.0135 (6)	−0.0024 (6)
S2B	0.0527 (11)	0.0488 (10)	0.0602 (12)	0.0017 (9)	0.0091 (9)	−0.0036 (9)
S3B	0.0219 (7)	0.0193 (6)	0.0240 (7)	0.0009 (6)	0.0018 (6)	−0.0022 (6)
P1B	0.0200 (7)	0.0178 (7)	0.0343 (8)	−0.0017 (6)	−0.0002 (6)	−0.0010 (6)
P2B	0.0204 (7)	0.0197 (7)	0.0239 (8)	0.0038 (6)	−0.0008 (6)	−0.0013 (6)
O1B	0.071 (4)	0.060 (3)	0.087 (4)	−0.010 (3)	−0.015 (3)	0.033 (3)
O2B	0.054 (3)	0.051 (3)	0.035 (3)	0.000 (2)	−0.010 (2)	0.000 (2)
N1B	0.030 (3)	0.022 (2)	0.036 (3)	0.003 (2)	0.010 (2)	−0.004 (2)
C1B	0.023 (3)	0.026 (3)	0.027 (3)	−0.005 (2)	−0.010 (2)	0.000 (2)
C2B	0.037 (3)	0.018 (3)	0.029 (3)	−0.008 (3)	−0.006 (3)	−0.006 (2)
C3B	0.027 (3)	0.018 (3)	0.023 (3)	0.002 (2)	−0.004 (2)	−0.001 (2)
C4B	0.017 (3)	0.033 (3)	0.026 (3)	−0.004 (3)	0.001 (2)	−0.005 (3)
C5B	0.034 (3)	0.030 (3)	0.038 (4)	−0.003 (3)	0.003 (3)	0.007 (3)
C6B	0.036 (4)	0.064 (4)	0.039 (4)	0.000 (3)	0.002 (3)	0.015 (3)
C7B	0.070 (5)	0.052 (4)	0.023 (4)	0.014 (4)	−0.002 (3)	0.005 (3)
C8B	0.083 (5)	0.031 (3)	0.034 (4)	−0.004 (4)	0.001 (4)	0.014 (3)
C9B	0.059 (4)	0.031 (3)	0.034 (4)	−0.005 (3)	0.000 (3)	−0.001 (3)
C10B	0.021 (3)	0.021 (3)	0.067 (5)	−0.007 (3)	0.005 (3)	−0.006 (3)
C11B	0.028 (3)	0.034 (3)	0.079 (5)	−0.002 (3)	−0.007 (3)	0.001 (3)
C12B	0.013 (3)	0.037 (4)	0.130 (7)	−0.005 (3)	−0.004 (4)	0.017 (4)
C13B	0.028 (4)	0.048 (4)	0.135 (8)	0.009 (3)	0.017 (4)	0.025 (5)
C14B	0.041 (4)	0.043 (4)	0.107 (6)	0.009 (3)	0.036 (4)	0.018 (4)
C15B	0.042 (4)	0.030 (3)	0.076 (5)	−0.006 (3)	0.025 (3)	0.007 (3)
C16B	0.020 (3)	0.025 (3)	0.018 (3)	−0.008 (2)	−0.001 (2)	0.003 (2)
C17B	0.021 (3)	0.022 (3)	0.037 (3)	0.005 (3)	−0.002 (3)	−0.003 (3)
C18B	0.027 (3)	0.029 (3)	0.043 (4)	0.000 (3)	−0.008 (3)	−0.004 (3)
C19B	0.021 (3)	0.042 (3)	0.034 (4)	−0.001 (3)	−0.004 (3)	0.010 (3)
C20B	0.030 (3)	0.025 (3)	0.045 (4)	0.008 (3)	−0.003 (3)	0.003 (3)
C21B	0.027 (3)	0.021 (3)	0.030 (3)	0.004 (2)	−0.002 (3)	−0.002 (3)
C22B	0.034 (3)	0.014 (3)	0.024 (3)	0.007 (2)	0.001 (2)	−0.001 (2)
C23B	0.036 (3)	0.032 (3)	0.030 (3)	0.005 (3)	0.008 (3)	0.003 (3)
C24B	0.035 (3)	0.032 (3)	0.049 (4)	−0.004 (3)	0.016 (3)	0.002 (3)
C25B	0.061 (4)	0.032 (3)	0.032 (4)	0.006 (3)	0.019 (3)	0.006 (3)
C26B	0.066 (4)	0.042 (4)	0.027 (4)	0.013 (4)	0.011 (3)	0.002 (3)
C27B	0.040 (3)	0.018 (3)	0.034 (4)	0.004 (3)	0.000 (3)	−0.006 (2)
C28B	0.037 (4)	0.068 (4)	0.088 (5)	−0.020 (4)	−0.026 (4)	0.041 (4)
C29B	0.026 (3)	0.026 (3)	0.083 (5)	−0.004 (3)	0.014 (3)	−0.003 (3)
C30B	0.066 (5)	0.032 (4)	0.108 (6)	0.018 (4)	−0.037 (4)	−0.017 (4)
C31B	0.091 (6)	0.035 (4)	0.064 (5)	0.003 (4)	0.015 (4)	0.004 (4)
C32B	0.086 (5)	0.078 (5)	0.030 (4)	0.036 (5)	0.002 (4)	0.023 (4)
C33B	0.048 (4)	0.014 (3)	0.017 (3)	0.001 (3)	0.005 (3)	0.005 (2)
C34B	0.027 (3)	0.021 (3)	0.048 (4)	−0.010 (3)	−0.007 (3)	0.015 (3)
C35B	0.040 (3)	0.024 (3)	0.028 (3)	−0.010 (3)	0.006 (3)	0.001 (3)
N2	0.091 (5)	0.217 (7)	0.172 (7)	0.084 (6)	−0.062 (5)	−0.147 (6)

N2B	0.067 (4)	0.124 (6)	0.086 (6)	0.049 (5)	0.001 (4)	−0.017 (5)
C36	0.071 (6)	0.126 (7)	0.089 (6)	−0.026 (6)	0.003 (5)	−0.056 (5)
C37	0.092 (6)	0.068 (4)	0.082 (6)	0.036 (5)	−0.018 (5)	−0.057 (4)
C36B	0.068 (6)	0.141 (9)	0.087 (7)	−0.009 (6)	−0.018 (5)	0.007 (7)
C37B	0.069 (5)	0.081 (5)	0.053 (5)	0.035 (5)	0.018 (4)	0.010 (4)

Geometric parameters (Å, º)

Ni—P1	2.2012 (14)	Ni1B—S1B	2.2495 (16)
Ni—P2	2.2060 (15)	Ni1B—S3B	2.2536 (14)
Ni—S3	2.2517 (13)	Ni1B—Cl1B	2.5971 (16)
Ni—S1	2.2574 (15)	Fe2B—C35B	1.760 (6)
Ni—Cl	2.5787 (14)	Fe2B—C34B	1.912 (7)
Fe—C35	1.759 (6)	Fe2B—N1B	2.065 (5)
Fe—C34	1.829 (6)	Fe2B—S2B	2.2839 (19)
Fe—N	2.048 (4)	Fe2B—S1B	2.2909 (16)
Fe—S1	2.2865 (15)	Fe2B—S3B	2.3029 (15)
Fe—S2	2.2978 (16)	S1B—C29B	1.821 (7)
Fe—S3	2.3159 (15)	S2B—C31B	1.844 (8)
S1—C29	1.838 (6)	S3B—C33B	1.803 (5)
S2—C31	1.831 (6)	P1B—C4B	1.810 (6)
S3—C33	1.811 (6)	P1B—C1B	1.812 (5)
P1—C4	1.825 (5)	P1B—C10B	1.833 (6)
P1—C10	1.839 (5)	P2B—C3B	1.818 (5)
P1—C1	1.841 (5)	P2B—C16B	1.830 (5)
P2—C3	1.807 (5)	P2B—C22B	1.833 (5)
P2—C22	1.825 (5)	O1B—C34B	0.861 (8)
P2—C16	1.834 (5)	O2B—C35B	1.137 (7)
O1—C34	1.065 (7)	N1B—C30B	1.471 (8)
O2—C35	1.151 (7)	N1B—C28B	1.488 (8)
N—C30	1.499 (6)	N1B—C32B	1.523 (8)
N—C32	1.508 (7)	C1B—C2B	1.529 (8)
N—C28	1.527 (7)	C1B—H1B1	0.99
C1—C2	1.505 (7)	C1B—H1B2	0.99
C1—H1A	0.99	C2B—C3B	1.549 (7)
C1—H1B	0.99	C2B—H2B1	0.99
C2—C3	1.533 (7)	C2B—H2B2	0.99
C2—H2A	0.99	C3B—H3B1	0.99
C2—H2B	0.99	C3B—H3B2	0.99
C3—H3A	0.99	C4B—C5B	1.367 (8)
C3—H3B	0.99	C4B—C9B	1.400 (8)
C4—C5	1.384 (7)	C5B—C6B	1.390 (8)
C4—C9	1.394 (8)	C5B—H5B	0.95
C5—C6	1.394 (8)	C6B—C7B	1.373 (9)
C5—H5	0.95	C6B—H6B	0.95
C6—C7	1.409 (9)	C7B—C8B	1.387 (10)
C6—H6	0.95	C7B—H7B	0.95
C7—C8	1.379 (9)	C8B—C9B	1.358 (9)

C7—H7	0.95	C8B—H8B	0.95
C8—C9	1.365 (8)	C9B—H9B	0.95
C8—H8	0.95	C10B—C15B	1.387 (9)
C9—H9	0.95	C10B—C11B	1.415 (9)
C10—C15	1.382 (7)	C11B—C12B	1.384 (9)
C10—C11	1.392 (8)	C11B—H11B	0.95
C11—C12	1.391 (8)	C12B—C13B	1.366 (12)
C11—H11	0.95	C12B—H12B	0.95
C12—C13	1.370 (9)	C13B—C14B	1.371 (11)
C12—H12	0.95	C13B—H13B	0.95
C13—C14	1.368 (8)	C14B—C15B	1.431 (9)
C13—H13	0.95	C14B—H14B	0.95
C14—C15	1.396 (8)	C15B—H15B	0.95
C14—H14	0.95	C16B—C21B	1.395 (7)
C15—H15	0.95	C16B—C17B	1.404 (7)
C16—C17	1.374 (7)	C17B—C18B	1.343 (8)
C16—C21	1.382 (7)	C17B—H17B	0.95
C17—C18	1.391 (8)	C18B—C19B	1.358 (8)
C17—H17	0.95	C18B—H18B	0.95
C18—C19	1.373 (8)	C19B—C20B	1.391 (8)
C18—H18	0.95	C19B—H19B	0.95
C19—C20	1.380 (8)	C20B—C21B	1.386 (8)
C19—H19	0.95	C20B—H20B	0.95
C20—C21	1.397 (8)	C21B—H21B	0.95
C20—H20	0.95	C22B—C23B	1.384 (8)
C21—H21	0.95	C22B—C27B	1.406 (8)
C22—C23	1.380 (8)	C23B—C24B	1.391 (8)
C22—C27	1.384 (8)	C23B—H23B	0.95
C23—C24	1.395 (8)	C24B—C25B	1.355 (9)
C23—H23	0.95	C24B—H24B	0.95
C24—C25	1.373 (9)	C25B—C26B	1.399 (9)
C24—H24	0.95	C25B—H25B	0.95
C25—C26	1.366 (9)	C26B—C27B	1.369 (9)
C25—H25	0.95	C26B—H26B	0.95
C26—C27	1.400 (8)	C27B—H27B	0.95
C26—H26	0.95	C28B—C29B	1.445 (9)
C27—H27	0.95	C28B—H28C	0.99
C28—C29	1.514 (8)	C28B—H28D	0.99
C28—H28A	0.99	C29B—H29C	0.99
C28—H28B	0.99	C29B—H29D	0.99
C29—H29A	0.99	C30B—C31B	1.591 (11)
C29—H29B	0.99	C30B—H30C	0.99
C30—C31	1.525 (8)	C30B—H30D	0.99
C30—H30A	0.99	C31B—H31C	0.99
C30—H30B	0.99	C31B—H31D	0.99
C31—H31A	0.99	C32B—C33B	1.464 (9)
C31—H31B	0.99	C32B—H32C	0.99
C32—C33	1.514 (8)	C32B—H32D	0.99

C32—H32A	0.99	C33B—H33C	0.99
C32—H32B	0.99	C33B—H33D	0.99
C33—H33A	0.99	N2—C37	1.160 (11)
C33—H33B	0.99	N2B—C37B	1.141 (11)
Ni1B—P1B	2.2018 (15)	C36—C37	1.462 (13)
Ni1B—P2B	2.2046 (15)	C36B—C37B	1.439 (12)

P1—Ni—P2	92.88 (5)	P1B—Ni1B—S1B	87.92 (6)
P1—Ni—S3	165.43 (6)	P2B—Ni1B—S1B	161.55 (6)
P2—Ni—S3	88.90 (5)	P1B—Ni1B—S3B	164.85 (6)
P1—Ni—S1	87.87 (5)	P2B—Ni1B—S3B	88.78 (5)
P2—Ni—S1	160.38 (6)	S1B—Ni1B—S3B	85.85 (5)
S3—Ni—S1	85.67 (5)	P1B—Ni1B—Cl1B	88.79 (5)
P1—Ni—Cl	88.51 (5)	P2B—Ni1B—Cl1B	92.29 (5)
P2—Ni—Cl	92.94 (5)	S1B—Ni1B—Cl1B	106.16 (6)
S3—Ni—Cl	105.85 (5)	S3B—Ni1B—Cl1B	106.21 (5)
S1—Ni—Cl	106.68 (5)	C35B—Fe2B—C34B	90.1 (3)
C35—Fe—C34	91.6 (2)	C35B—Fe2B—N1B	177.9 (2)
C35—Fe—N	175.2 (2)	C34B—Fe2B—N1B	91.8 (2)
C34—Fe—N	92.5 (2)	C35B—Fe2B—S2B	94.41 (19)
C35—Fe—S1	95.72 (19)	C34B—Fe2B—S2B	87.86 (18)
C34—Fe—S1	96.10 (18)	N1B—Fe2B—S2B	86.57 (13)
N—Fe—S1	86.26 (12)	C35B—Fe2B—S1B	92.44 (18)
C35—Fe—S2	90.91 (19)	C34B—Fe2B—S1B	95.97 (18)
C34—Fe—S2	87.63 (18)	N1B—Fe2B—S1B	86.47 (13)
N—Fe—S2	86.83 (12)	S2B—Fe2B—S1B	172.15 (7)
S1—Fe—S2	172.29 (7)	C35B—Fe2B—S3B	90.78 (19)
C35—Fe—S3	88.34 (18)	C34B—Fe2B—S3B	179.1 (2)
C34—Fe—S3	179.60 (19)	N1B—Fe2B—S3B	87.29 (13)
N—Fe—S3	87.58 (12)	S2B—Fe2B—S3B	92.30 (6)
S1—Fe—S3	83.53 (5)	S1B—Fe2B—S3B	83.76 (5)
S2—Fe—S3	92.76 (6)	C29B—S1B—Ni1B	106.3 (2)
C29—S1—Ni	105.5 (2)	C29B—S1B—Fe2B	99.02 (19)
C29—S1—Fe	99.79 (18)	Ni1B—S1B—Fe2B	95.18 (6)
Ni—S1—Fe	95.51 (6)	C31B—S2B—Fe2B	98.7 (2)
C31—S2—Fe	98.65 (18)	C33B—S3B—Ni1B	108.53 (19)
C33—S3—Ni	109.84 (18)	C33B—S3B—Fe2B	97.50 (18)
C33—S3—Fe	96.70 (17)	Ni1B—S3B—Fe2B	94.74 (5)
Ni—S3—Fe	94.85 (5)	C4B—P1B—C1B	103.1 (2)
C4—P1—C10	104.3 (2)	C4B—P1B—C10B	103.2 (3)
C4—P1—C1	103.2 (2)	C1B—P1B—C10B	103.0 (3)
C10—P1—C1	101.9 (2)	C4B—P1B—Ni1B	114.42 (18)
C4—P1—Ni	113.45 (17)	C1B—P1B—Ni1B	115.71 (18)
C10—P1—Ni	116.11 (16)	C10B—P1B—Ni1B	115.63 (19)
C1—P1—Ni	116.24 (18)	C3B—P2B—C16B	105.9 (2)
C3—P2—C22	101.7 (2)	C3B—P2B—C22B	102.3 (2)
C3—P2—C16	105.9 (2)	C16B—P2B—C22B	103.9 (2)
C22—P2—C16	104.3 (2)	C3B—P2B—Ni1B	116.50 (18)

C3—P2—Ni	115.61 (18)	C16B—P2B—Ni1B	111.67 (17)
C22—P2—Ni	115.54 (17)	C22B—P2B—Ni1B	115.26 (17)
C16—P2—Ni	112.53 (17)	C30B—N1B—C28B	108.2 (5)
C30—N—C32	110.8 (4)	C30B—N1B—C32B	112.5 (5)
C30—N—C28	106.6 (4)	C28B—N1B—C32B	103.2 (5)
C32—N—C28	105.9 (4)	C30B—N1B—Fe2B	109.8 (4)
C30—N—Fe	109.4 (3)	C28B—N1B—Fe2B	109.3 (4)
C32—N—Fe	114.3 (3)	C32B—N1B—Fe2B	113.5 (4)
C28—N—Fe	109.4 (3)	C2B—C1B—P1B	114.5 (4)
C2—C1—P1	114.5 (4)	C2B—C1B—H1B1	108.6
C2—C1—H1A	108.6	P1B—C1B—H1B1	108.6
P1—C1—H1A	108.6	C2B—C1B—H1B2	108.6
C2—C1—H1B	108.6	P1B—C1B—H1B2	108.6
P1—C1—H1B	108.6	H1B1—C1B—H1B2	107.6
H1A—C1—H1B	107.6	C1B—C2B—C3B	114.4 (4)
C1—C2—C3	113.5 (4)	C1B—C2B—H2B1	108.7
C1—C2—H2A	108.9	C3B—C2B—H2B1	108.7
C3—C2—H2A	108.9	C1B—C2B—H2B2	108.7
C1—C2—H2B	108.9	C3B—C2B—H2B2	108.7
C3—C2—H2B	108.9	H2B1—C2B—H2B2	107.6
H2A—C2—H2B	107.7	C2B—C3B—P2B	114.7 (4)
C2—C3—P2	115.9 (4)	C2B—C3B—H3B1	108.6
C2—C3—H3A	108.3	P2B—C3B—H3B1	108.6
P2—C3—H3A	108.3	C2B—C3B—H3B2	108.6
C2—C3—H3B	108.3	P2B—C3B—H3B2	108.6
P2—C3—H3B	108.3	H3B1—C3B—H3B2	107.6
H3A—C3—H3B	107.4	C5B—C4B—C9B	116.8 (5)
C5—C4—C9	118.9 (5)	C5B—C4B—P1B	121.2 (4)
C5—C4—P1	121.0 (4)	C9B—C4B—P1B	121.9 (4)
C9—C4—P1	120.0 (4)	C4B—C5B—C6B	122.0 (6)
C4—C5—C6	120.6 (6)	C4B—C5B—H5B	119
C4—C5—H5	119.7	C6B—C5B—H5B	119
C6—C5—H5	119.7	C7B—C6B—C5B	120.2 (6)
C5—C6—C7	118.5 (6)	C7B—C6B—H6B	119.9
C5—C6—H6	120.7	C5B—C6B—H6B	119.9
C7—C6—H6	120.7	C6B—C7B—C8B	118.2 (6)
C8—C7—C6	120.6 (6)	C6B—C7B—H7B	120.9
C8—C7—H7	119.7	C8B—C7B—H7B	120.9
C6—C7—H7	119.7	C9B—C8B—C7B	121.0 (6)
C9—C8—C7	119.7 (6)	C9B—C8B—H8B	119.5
C9—C8—H8	120.2	C7B—C8B—H8B	119.5
C7—C8—H8	120.2	C8B—C9B—C4B	121.6 (6)
C8—C9—C4	121.4 (6)	C8B—C9B—H9B	119.2
C8—C9—H9	119.3	C4B—C9B—H9B	119.2
C4—C9—H9	119.3	C15B—C10B—C11B	120.5 (6)
C15—C10—C11	119.1 (5)	C15B—C10B—P1B	119.9 (5)
C15—C10—P1	121.6 (4)	C11B—C10B—P1B	119.5 (5)
C11—C10—P1	119.3 (4)	C12B—C11B—C10B	120.1 (7)

C10—C11—C12	119.5 (5)	C12B—C11B—H11B	120
C10—C11—H11	120.2	C10B—C11B—H11B	120
C12—C11—H11	120.2	C13B—C12B—C11B	119.2 (7)
C13—C12—C11	121.0 (5)	C13B—C12B—H12B	120.4
C13—C12—H12	119.5	C11B—C12B—H12B	120.4
C11—C12—H12	119.5	C12B—C13B—C14B	122.5 (7)
C14—C13—C12	119.6 (5)	C12B—C13B—H13B	118.7
C14—C13—H13	120.2	C14B—C13B—H13B	118.7
C12—C13—H13	120.2	C13B—C14B—C15B	119.6 (8)
C13—C14—C15	120.4 (6)	C13B—C14B—H14B	120.2
C13—C14—H14	119.8	C15B—C14B—H14B	120.2
C15—C14—H14	119.8	C10B—C15B—C14B	118.0 (7)
C10—C15—C14	120.3 (5)	C10B—C15B—H15B	121
C10—C15—H15	119.9	C14B—C15B—H15B	121
C14—C15—H15	119.9	C21B—C16B—C17B	118.3 (5)
C17—C16—C21	119.1 (5)	C21B—C16B—P2B	122.9 (4)
C17—C16—P2	118.8 (4)	C17B—C16B—P2B	118.7 (4)
C21—C16—P2	121.9 (4)	C18B—C17B—C16B	120.7 (5)
C16—C17—C18	121.3 (5)	C18B—C17B—H17B	119.7
C16—C17—H17	119.4	C16B—C17B—H17B	119.7
C18—C17—H17	119.4	C17B—C18B—C19B	121.9 (6)
C19—C18—C17	119.0 (5)	C17B—C18B—H18B	119
C19—C18—H18	120.5	C19B—C18B—H18B	119
C17—C18—H18	120.5	C18B—C19B—C20B	119.1 (5)
C18—C19—C20	120.9 (5)	C18B—C19B—H19B	120.5
C18—C19—H19	119.6	C20B—C19B—H19B	120.5
C20—C19—H19	119.6	C21B—C20B—C19B	120.4 (5)
C19—C20—C21	119.4 (5)	C21B—C20B—H20B	119.8
C19—C20—H20	120.3	C19B—C20B—H20B	119.8
C21—C20—H20	120.3	C20B—C21B—C16B	119.6 (5)
C16—C21—C20	120.3 (5)	C20B—C21B—H21B	120.2
C16—C21—H21	119.9	C16B—C21B—H21B	120.2
C20—C21—H21	119.9	C23B—C22B—C27B	118.4 (5)
C23—C22—C27	119.2 (5)	C23B—C22B—P2B	122.2 (4)
C23—C22—P2	122.0 (4)	C27B—C22B—P2B	119.3 (4)
C27—C22—P2	118.8 (4)	C22B—C23B—C24B	119.9 (6)
C22—C23—C24	120.7 (5)	C22B—C23B—H23B	120.1
C22—C23—H23	119.7	C24B—C23B—H23B	120.1
C24—C23—H23	119.7	C25B—C24B—C23B	121.7 (6)
C25—C24—C23	119.5 (6)	C25B—C24B—H24B	119.1
C25—C24—H24	120.2	C23B—C24B—H24B	119.1
C23—C24—H24	120.2	C24B—C25B—C26B	118.9 (6)
C26—C25—C24	120.6 (6)	C24B—C25B—H25B	120.6
C26—C25—H25	119.7	C26B—C25B—H25B	120.6
C24—C25—H25	119.7	C27B—C26B—C25B	120.4 (6)
C25—C26—C27	120.0 (6)	C27B—C26B—H26B	119.8
C25—C26—H26	120	C25B—C26B—H26B	119.8
C27—C26—H26	120	C26B—C27B—C22B	120.6 (6)

C22—C27—C26	120.0 (5)	C26B—C27B—H27B	119.7
C22—C27—H27	120	C22B—C27B—H27B	119.7
C26—C27—H27	120	C29B—C28B—N1B	117.8 (6)
C29—C28—N	111.9 (4)	C29B—C28B—H28C	107.9
C29—C28—H28A	109.2	N1B—C28B—H28C	107.9
N—C28—H28A	109.2	C29B—C28B—H28D	107.9
C29—C28—H28B	109.2	N1B—C28B—H28D	107.9
N—C28—H28B	109.2	H28C—C28B—H28D	107.2
H28A—C28—H28B	107.9	C28B—C29B—S1B	113.7 (5)
C28—C29—S1	111.9 (4)	C28B—C29B—H29C	108.8
C28—C29—H29A	109.2	S1B—C29B—H29C	108.8
S1—C29—H29A	109.2	C28B—C29B—H29D	108.8
C28—C29—H29B	109.2	S1B—C29B—H29D	108.8
S1—C29—H29B	109.2	H29C—C29B—H29D	107.7
H29A—C29—H29B	107.9	N1B—C30B—C31B	106.4 (5)
N—C30—C31	109.8 (4)	N1B—C30B—H30C	110.5
N—C30—H30A	109.7	C31B—C30B—H30C	110.5
C31—C30—H30A	109.7	N1B—C30B—H30D	110.5
N—C30—H30B	109.7	C31B—C30B—H30D	110.5
C31—C30—H30B	109.7	H30C—C30B—H30D	108.6
H30A—C30—H30B	108.2	C30B—C31B—S2B	108.4 (5)
C30—C31—S2	109.7 (4)	C30B—C31B—H31C	110
C30—C31—H31A	109.7	S2B—C31B—H31C	110
S2—C31—H31A	109.7	C30B—C31B—H31D	110
C30—C31—H31B	109.7	S2B—C31B—H31D	110
S2—C31—H31B	109.7	H31C—C31B—H31D	108.4
H31A—C31—H31B	108.2	C33B—C32B—N1B	115.4 (5)
N—C32—C33	114.1 (5)	C33B—C32B—H32C	108.4
N—C32—H32A	108.7	N1B—C32B—H32C	108.4
C33—C32—H32A	108.7	C33B—C32B—H32D	108.4
N—C32—H32B	108.7	N1B—C32B—H32D	108.4
C33—C32—H32B	108.7	H32C—C32B—H32D	107.5
H32A—C32—H32B	107.6	C32B—C33B—S3B	112.3 (4)
C32—C33—S3	110.6 (4)	C32B—C33B—H33C	109.1
C32—C33—H33A	109.5	S3B—C33B—H33C	109.1
S3—C33—H33A	109.5	C32B—C33B—H33D	109.1
C32—C33—H33B	109.5	S3B—C33B—H33D	109.1
S3—C33—H33B	109.5	H33C—C33B—H33D	107.9
H33A—C33—H33B	108.1	O1B—C34B—Fe2B	175.4 (8)
O1—C34—Fe	175.3 (5)	O2B—C35B—Fe2B	176.9 (5)
O2—C35—Fe	176.9 (5)	N2—C37—C36	175.4 (9)
P1B—Ni1B—P2B	92.84 (6)	N2B—C37B—C36B	178.0 (10)

Fe—S1—C29—C28	−9.4 (6)	C29B—C28B—N1B—Fe2B	−43.0 (10)
S1—C29—C28—N	38.6 (8)	Fe2B—S2B—C31B—C30B	25.8 (8)
C29—C28—N—Fe	−51.9 (7)	S2B—C31B—C30B—N1B	−54.9 (10)
Fe—S2—C31—C30	23.7 (6)	C31B—C30B—N1B—Fe2B	58.7 (9)
S2—C31—C30—N	−51.7 (8)	Fe2B—S3B—C33B—C32B	−35.8 (7)

C31—C30—N—Fe	55.3 (7)	S3B—C33B—C32B—N1B	42.1 (10)
Fe—S3—C33—C32	−38.3 (6)	C33B—C32B—N1B—Fe2B	−24.5 (10)
S3—C33—C32—N	45.8 (8)	P1—C1—C2—C3	−68.5 (8)
C33—C32—N—Fe	−27.3 (8)	C1—C2—C3—P2	69.7 (8)
Fe2B—S1B—C29B—C28B	−3.0 (8)	P1B—C1B—C2B—C3B	−69.3 (8)
S1B—C29B—C28B—N1B	29.6 (12)	C1B—C2B—C3B—P2B	67.1 (8)