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1,3-Bis(diphenylphosphino)propane-2κ^2P,P'-{μ-2-[bis(2-mercaptoethyl)amino]ethanesulfinato(3–)-1κ^4N,S,S',S'':2κ^2S,S'}chloro-2κCl-dinitroso-1κ^2N-iron(II)nickel(II) acetonitrile hemisolvate

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Key indicators

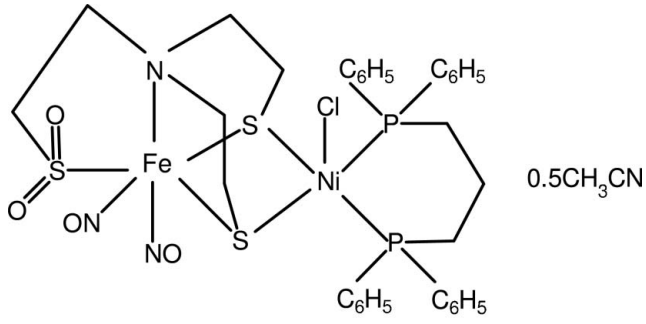
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.019 Å
H-atom completeness 97%
R factor = 0.108
wR factor = 0.256
Data-to-parameter ratio = 30.5

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

The title compound, [{Fe[$(SO_2CH_2CH_2)(SCH_2CH_2)_2N$]-$(NO)_2$-*S*,*S*'}NiCl{[$P(C_6H_5)_2]_2(CH_2)_3$}]·0.5$CH_3CN$ or [Fe-Ni$(C_6H_{12}NO_2S_3)Cl(C_{27}H_{26}P_2)(NO)_2$]·0.5$C_2H_3N$, is described. There are two crystallographically distinct dimetallic complex molecules. In each molecule, the Fe atom is octahedrally coordinated, with the three S atoms and an N atom of one of the two NO ligands forming the equatorial plane; the N atoms from the second NO group and the $(SO_2CH_2CH_2)$-$(SCH_2CH_2)_2N$ ligand lie in the axial positions. The Ni atom is square pyramidally coordinated by the two bridging S atoms and the two P atoms forming the basal plane, and by the Cl atom lying in the apical position. Slight differences in the bonding modes of the NO ligands are observed for the two distinct molecules.

Comment

As part of our studies on the synthesis of dimetallic complexes with structural properties related to the active site of the enzyme nickel–iron hydrogenase (Evans & Pickett, 2003), we have been exploring the utility of the anion $[Fe\{(SCH_2CH_2)_3N\}(NO)]^-$ as a synthon (Davies *et al.*, 2002; Smith *et al.*, 2002; Smith *et al.*, 2003). The title compound, (I), crystallized as an unexpected minor product after long-term storage of a solution in acetonitrile at 277 K, from the attempted preparation of [{Fe[$(SCH_2CH_2)_3N$](NO)-*S*,*S*'}NiCl-{[$P(C_6H_5)_2]_2(CH_2)_3$}] following an adaptation of the method established for a related complex (Smith *et al.*, 2002).



(I)

The asymmetric unit of (I) contains two complex molecules, denoted *A* (containing Fe and Ni) and *B* (Fe1*b* and Ni1*b*), and one CH_3CN solvent molecule, the latter showing signs of disorder (Fig. 1).

The structures of *A* and *B* in (I) closely resemble those of the analogous species in [{Fe[$(SCH_2CH_2)_3N$]$(CO)_2$-*S*,*S*'}NiCl{[$P(C_6H_5)_2]_2(CH_2)_3$}], (II) (Duff *et al.*, 2005), with bond dimensions similar in both. In (I), both Fe atoms are

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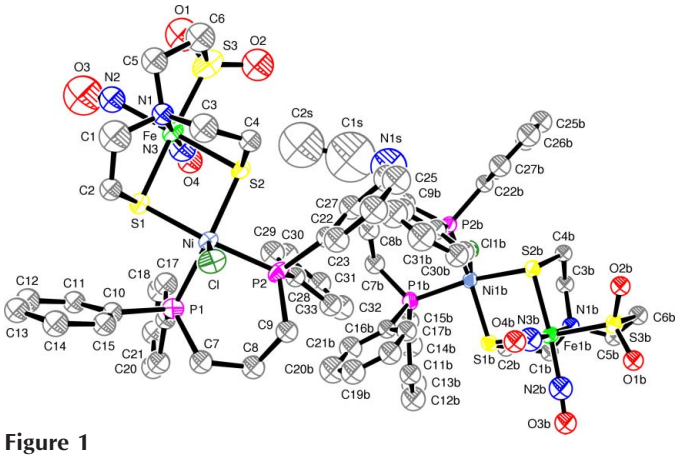

Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids (H atoms have been omitted for clarity).

octahedrally coordinated, with the three S atoms and the N atom of one of the NO ligands forming the equatorial plane, while the N atoms from the $(SO_2CH_2CH_2)(SCH_2CH_2)_2N$ and second NO ligand lie in the axial positions. The Fe atoms lie 0.119 (2) and 0.045 (2) Å from the mean equatorial planes in molecules *A* and *B*, respectively, and are displaced towards the axial NO ligands. The Ni atoms are square pyramidally coordinated with an S_2P_2 base plane and the Cl atom lying in the apical position. The Ni atoms lie 0.297 (2) and 0.328 (2) Å from the mean base planes for molecules *A* and *B*, respectively, displaced towards the Cl atoms. The angle between the normals to the mean equatorial and base planes are 167.35 (8) and 159.69 (8)° for *A* and *B*, respectively, with Fe···Ni distances of 3.372 (2) and 3.343 (2) Å.

Bond distances about the metal atoms are not unusual (Table 1); within the core of the $(SO_2CH_2CH_2)(SCH_2CH_2)_2N$ ligand and in the $[P(C_6H_5)_2]_2(CH_2)_3$ ligand, dimensions are as found in (II), including the removal of the usual pseudo-threefold rotation about the *M*—N axis of $(SCH_2CH_2)_3N$ and related ligands by the non-bridging SCH_2CH_2 group. Three of the NO ligands are classed as being 'linear' (Table 2), while the equatorial NO in molecule *A* may be described as 'bent'. The configuration is different in (II), where both CO ligands in the two independent molecules are linear, as expected, with *M*—C—O bond angles of 175.3 (5) and 176.9 (5)° in one molecule, and 175.4 (8) and 176.9 (5) Å in the second.

The component molecules in (I) are arranged within the crystal structure with normal van der Waals contacts between the individual components.

Experimental

Under a dinitrogen atmosphere, $(NEt_4)[Fe\{(SCH_2CH_2)_3N\}(NO)]$ (0.12 g, 0.29 mmol) was added to a stirred solution of $[NiCl_2(dppp)]$ (0.16 g, 0.29 mmol) in MeCN (75 ml). The reaction mixture was stirred overnight. Some red–brown precipitate was removed by filtration and the filtrate stored for eight months at 277 K. After this time, a few red crystals of (I) were collected by filtration. ν(NO), KBr: 1704 and 1733 cm^{-1}; Mössbauer (solid, 80 K, relative to iron foil at 298 K) isomer shift 0.26 mm s^{-1}, quadrupole splitting 1.19 mm s^{-1}.

Crystal data

$[FeNi(C_6H_{12}NO_2S_3)Cl(C_{27}H_{26}P_2)(NO)_2]\cdot 0.5C_2H_3N$
M_r = 869.32
Monoclinic, $P2_1/n$
a = 16.5125 (5) Å
b = 17.8156 (6) Å
c = 25.5801 (8) Å
β = 99.913 (2)°
V = 7412.8 (4) Å^3
Z = 8
D_x = 1.558 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 52202 reflections
θ = 3.4–26.0°
μ = 1.27 mm^{-1}
T = 173 (2) K
Prism, red
0.10 × 0.05 × 0.02 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.864, T_{max} = 0.975
52202 measured reflections
14540 independent reflections
7005 reflections with $I > 2\sigma(I)$
R_{int} = 0.155
θ_{max} = 26.0°
$h = -20 \rightarrow 18$
$k = -20 \rightarrow 21$
$l = -31 \rightarrow 31$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.108
$wR(F^2)$ = 0.256
S = 0.99
14540 reflections
477 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2 + 96.5506P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 1.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.79 e Å^{-3}

Table 1
Selected interatomic distances (Å).

Ni—S1	2.248 (3)	Ni1*b*—S1*b*	2.253 (3)
Ni—S2	2.243 (3)	Ni1*b*—S2*b*	2.259 (3)
Ni—P1	2.205 (3)	Ni1*b*—P1*b*	2.193 (3)
Ni—P2	2.201 (3)	Ni1*b*—P2*b*	2.203 (3)
Ni—Cl	2.607 (3)	Ni1*b*—Cl1*b*	2.560 (3)
Fe—N1	2.039 (9)	Fe1*b*—N1*b*	2.052 (9)
Fe—N2	1.991 (12)	Fe1*b*—N2*b*	1.794 (12)
Fe—N3	1.760 (12)	Fe1*b*—N3*b*	1.781 (12)
Fe—S1	2.305 (3)	Fe1*b*—S1*b*	2.290 (3)
Fe—S2	2.284 (3)	Fe1*b*—S2*b*	2.293 (3)
Fe—S3	2.222 (5)	Fe1*b*—S3*b*	2.224 (3)

Table 2
Bond lengths (Å) and angles (°) in idealized NO ligands and in complex (I).

			Molecule *A*		Molecule *B*	
	Bent	Linear	Equatorial	Axial	Equatorial	Axial
M—N—O	149	175	149.1 (14)	175.1 (10)	176.4 (10)	177.3 (10)
M—N	1.992	1.759	1.991 (12)	1.759 (12)	1.779 (12)	1.794 (12)
N—O	1.023	1.177	1.023 (16)	1.177 (12)	1.157 (12)	1.158 (12)

The crystal of (I) was a very weak scatterer, particularly at higher angles. All C, N and O atoms were refined isotropically. H atoms were positioned geometrically (C—H = 0.95–0.99 Å) and refined as riding [U_{iso}(H) = 1.2U_{eq}(C)]. The H atoms of the solvent molecule were not located. The highest peak is located 0.96 Å from atom O3.

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: *SHELXS86* (Sheldrick, 1986); 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**, m1313–m1315 [https://doi.org/10.1107/S1600536805018027]

1,3-Bis(diphenylphosphino)propane-2κ^2P,P'-{μ-2-[bis(2-mercaptoethyl)amino]-ethanesulfinato(3–)-1κ^4N,S,S',S'':2κ^2S,S'}chloro-2κCl-dinitroso-1κ^2N-iron(II)nickel(II) acetonitrile hemisolvate

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(I)

Crystal data

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Hall symbol: -P 2yn
$a = 16.5125$ (5) Å
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$\beta = 99.913$ (2)°
$V = 7412.8$ (4) Å^3
$Z = 8$
$F(000) = 3592$
$D_x = 1.558$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 89254 reflections
$\theta = 3.4$–26.0°
$\mu = 1.27$ mm^{-1}
$T = 173$ K
Prism, red
0.10 × 0.05 × 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 (SORTAV; Blessing, 1995)
$T_{min} = 0.864$, $T_{max} = 0.975$
52202 measured reflections
14540 independent reflections
7005 reflections with $I > 2\sigma(I)$
$R_{int} = 0.155$
$\theta_{max} = 26.0°$, $\theta_{min} = 3.4°$
$h = -20\rightarrow 18$
$k = -20\rightarrow 21$
$l = -31\rightarrow 31$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.108$
$wR(F^2) = 0.256$
$S = 0.99$
14540 reflections
477 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
$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2 + 96.5506P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 1.63$ e Å^{-3}
$\Delta\rho_{min} = -0.79$ 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. ********** The diffraction was very weak, particularly at higher angle. But this was the best (or least bad !) crystal available. **********

C,*N*, and O atoms had to be left isotropic otherwise some went non-positive-definite. The H atoms for the CH3CN solvate molecule were omitted.

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	0.82086 (8)	0.06690 (8)	0.10598 (5)	0.0284 (3)
Fe	0.71629 (9)	−0.00387 (9)	−0.00821 (6)	0.0323 (4)
Cl	0.97792 (17)	0.03802 (17)	0.12602 (11)	0.0429 (7)
S1	0.79207 (16)	0.10157 (15)	0.02032 (10)	0.0306 (6)
S2	0.75690 (17)	−0.04049 (15)	0.07790 (10)	0.0308 (6)
S3	0.6562 (2)	−0.1130 (2)	−0.03239 (14)	0.0645 (11)
P1	0.84817 (17)	0.18479 (16)	0.12867 (11)	0.0320 (7)
P2	0.81271 (18)	0.03457 (17)	0.18795 (11)	0.0336 (7)
O1	0.5937 (7)	−0.1071 (7)	−0.0801 (5)	0.096 (4)*
O2	0.6323 (7)	−0.1606 (6)	0.0087 (4)	0.087 (3)*
O3	0.6667 (9)	0.0603 (9)	−0.1138 (6)	0.134 (5)*
O4	0.5668 (5)	0.0589 (5)	0.0222 (3)	0.055 (2)*
N1	0.8235 (5)	−0.0473 (5)	−0.0245 (3)	0.036 (2)*
N2	0.6952 (7)	0.0256 (6)	−0.0845 (5)	0.056 (3)*
N3	0.6249 (7)	0.0332 (6)	0.0078 (4)	0.063 (3)*
C1	0.8715 (10)	0.0161 (9)	−0.0442 (6)	0.080 (5)*
H1A	0.9262	−0.0032	−0.0484	0.096*
H1B	0.8426	0.0316	−0.0797	0.096*
C2	0.8833 (7)	0.0835 (6)	−0.0094 (4)	0.038 (3)*
H2A	0.8946	0.1277	−0.0304	0.045*
H2B	0.9313	0.0757	0.0191	0.045*
C3	0.8724 (9)	−0.0865 (8)	0.0208 (5)	0.064 (4)*
H3A	0.8945	−0.1327	0.0071	0.077*
H3B	0.9201	−0.0541	0.0346	0.077*
C4	0.8339 (7)	−0.1079 (6)	0.0657 (4)	0.038 (3)*
H4A	0.8766	−0.1122	0.0978	0.046*
H4B	0.8077	−0.1578	0.0587	0.046*
C5	0.8048 (8)	−0.0998 (7)	−0.0702 (5)	0.053 (3)*
H5A	0.8558	−0.1236	−0.0776	0.064*
H5B	0.7781	−0.0728	−0.1024	0.064*
C6	0.7446 (9)	−0.1610 (8)	−0.0534 (6)	0.067 (4)*

H6A	0.774	−0.1917	−0.0239	0.08*
H6B	0.7251	−0.1947	−0.0837	0.08*
C7	0.9129 (7)	0.2016 (7)	0.1926 (4)	0.043 (3)*
H7A	0.9689	0.1825	0.1914	0.051*
H7B	0.9173	0.2564	0.1988	0.051*
C8	0.8811 (7)	0.1644 (6)	0.2401 (5)	0.044 (3)*
H8A	0.9131	0.1838	0.2737	0.052*
H8B	0.8228	0.1785	0.239	0.052*
C9	0.8881 (7)	0.0788 (6)	0.2396 (4)	0.039 (3)*
H9A	0.8806	0.0591	0.2746	0.047*
H9B	0.944	0.0649	0.234	0.047*
C10	0.9019 (7)	0.2354 (6)	0.0825 (4)	0.034 (3)*
C11	0.8592 (7)	0.2787 (6)	0.0423 (4)	0.039 (3)*
H11	0.8019	0.2869	0.0405	0.047*
C12	0.8998 (7)	0.3103 (7)	0.0045 (5)	0.047 (3)*
H12	0.8696	0.3394	−0.0234	0.057*
C13	0.9838 (7)	0.3004 (7)	0.0066 (5)	0.047 (3)*
H13	1.0109	0.3207	−0.0201	0.057*
C14	1.0268 (8)	0.2601 (7)	0.0485 (5)	0.051 (3)*
H14	1.0847	0.2553	0.0517	0.061*
C15	0.9866 (7)	0.2264 (6)	0.0864 (5)	0.040 (3)*
H15	1.0168	0.1976	0.1144	0.048*
C16	0.7570 (6)	0.2409 (6)	0.1302 (4)	0.033 (3)*
C17	0.6815 (7)	0.2184 (7)	0.1017 (5)	0.047 (3)*
H17	0.6787	0.1727	0.0823	0.056*
C18	0.6099 (8)	0.2599 (7)	0.1004 (5)	0.054 (4)*
H18	0.5595	0.2436	0.0798	0.065*
C19	0.6137 (8)	0.3252 (7)	0.1296 (5)	0.052 (3)*
H19	0.5653	0.3539	0.1299	0.063*
C20	0.6856 (8)	0.3484 (7)	0.1577 (5)	0.050 (3)*
H20	0.6873	0.3937	0.1774	0.06*
C21	0.7575 (7)	0.3078 (6)	0.1586 (5)	0.044 (3)*
H21	0.8075	0.3256	0.1788	0.052*
C22	0.8274 (7)	−0.0663 (6)	0.2007 (4)	0.036 (3)*
C23	0.9082 (8)	−0.0960 (7)	0.2092 (5)	0.048 (3)*
H23	0.9547	−0.0643	0.2103	0.058*
C24	0.9170 (9)	−0.1736 (8)	0.2159 (5)	0.059 (4)*
H24	0.9705	−0.1949	0.2226	0.071*
C25	0.8530 (9)	−0.2172 (9)	0.2129 (5)	0.064 (4)*
H25	0.8616	−0.2698	0.216	0.077*
C26	0.7718 (9)	−0.1900 (8)	0.2055 (5)	0.060 (4)*
H26	0.7263	−0.2226	0.2053	0.072*
C27	0.7616 (8)	−0.1122 (7)	0.1983 (5)	0.047 (3)*
H27	0.7077	−0.0916	0.1917	0.056*
C28	0.7147 (6)	0.0533 (6)	0.2075 (4)	0.033 (3)*
C29	0.6469 (8)	0.0667 (7)	0.1690 (5)	0.051 (3)*
H29	0.6523	0.0672	0.1326	0.061*
C30	0.5692 (9)	0.0796 (8)	0.1838 (6)	0.062 (4)*

H30	0.522	0.0872	0.1573	0.074*
C31	0.5620 (8)	0.0812 (7)	0.2369 (5)	0.050 (3)*
H31	0.5103	0.0911	0.2469	0.06*
C32	0.6289 (8)	0.0687 (7)	0.2744 (5)	0.055 (3)*
H32	0.624	0.0695	0.3109	0.066*
C33	0.7036 (7)	0.0548 (6)	0.2603 (5)	0.042 (3)*
H33	0.7496	0.0458	0.2874	0.051*
Ni1B	0.18700 (8)	−0.00349 (8)	0.38970 (5)	0.0299 (3)
Fe1B	0.27592 (9)	−0.04471 (9)	0.51387 (6)	0.0289 (4)
Cl1B	0.02994 (16)	−0.01142 (15)	0.36928 (11)	0.0375 (7)
S1B	0.21976 (16)	0.05808 (15)	0.46740 (11)	0.0319 (7)
S2B	0.22663 (16)	−0.10827 (15)	0.43699 (10)	0.0306 (6)
S3B	0.31347 (17)	−0.14938 (16)	0.55897 (11)	0.0346 (7)
P1B	0.17828 (18)	0.10730 (17)	0.35174 (12)	0.0361 (7)
P2B	0.20497 (18)	−0.06121 (18)	0.31640 (11)	0.0354 (7)
O1B	0.3755 (5)	−0.1349 (4)	0.6061 (3)	0.042 (2)*
O2B	0.3299 (4)	−0.2145 (4)	0.5280 (3)	0.0401 (19)*
O3B	0.3461 (5)	0.0478 (5)	0.6063 (3)	0.052 (2)*
O4B	0.4305 (5)	−0.0315 (5)	0.4724 (3)	0.049 (2)*
N1B	0.1625 (5)	−0.0575 (5)	0.5352 (3)	0.032 (2)*
N2B	0.3173 (7)	0.0101 (6)	0.5711 (5)	0.061 (3)*
N3B	0.3706 (7)	−0.0372 (6)	0.4899 (4)	0.059 (3)*
C1B	0.1286 (7)	0.0187 (6)	0.5439 (4)	0.037 (3)*
H1B1	0.1632	0.0425	0.575	0.044*
H1B2	0.0724	0.0131	0.5521	0.044*
C2B	0.1254 (7)	0.0694 (6)	0.4961 (4)	0.036 (3)*
H2B1	0.12	0.1223	0.5068	0.043*
H2B2	0.0769	0.0565	0.4691	0.043*
C3B	0.1003 (7)	−0.0984 (6)	0.4937 (4)	0.037 (3)*
H3B1	0.0625	−0.1274	0.5122	0.044*
H3B2	0.0671	−0.0607	0.4711	0.044*
C4B	0.1380 (6)	−0.1508 (6)	0.4589 (4)	0.033 (3)*
H4B1	0.0965	−0.1642	0.4276	0.04*
H4B2	0.1552	−0.1975	0.4787	0.04*
C5B	0.1720 (7)	−0.0990 (6)	0.5873 (4)	0.039 (3)*
H5B1	0.117	−0.1103	0.5958	0.047*
H5B2	0.2017	−0.0669	0.6159	0.047*
C6B	0.2189 (7)	−0.1714 (6)	0.5847 (5)	0.040 (3)*
H6B1	0.185	−0.2076	0.561	0.047*
H6B2	0.2326	−0.194	0.6205	0.047*
C7B	0.1237 (7)	0.1110 (7)	0.2837 (5)	0.047 (3)*
H7B1	0.0652	0.0986	0.2835	0.057*
H7B2	0.126	0.1631	0.2705	0.057*
C8B	0.1579 (8)	0.0574 (7)	0.2452 (5)	0.049 (3)*
H8B1	0.1316	0.0693	0.2083	0.059*
H8B2	0.2177	0.066	0.248	0.059*
C9B	0.1431 (7)	−0.0249 (7)	0.2563 (5)	0.045 (3)*
H9B1	0.1544	−0.0551	0.2259	0.054*

H9B2	0.0844	−0.0316	0.2587	0.054*
C10B	0.1254 (7)	0.1765 (6)	0.3853 (5)	0.041 (3)*
C11B	0.1666 (8)	0.2245 (7)	0.4237 (5)	0.053 (3)*
H11B	0.225	0.225	0.4296	0.064*
C12B	0.1260 (10)	0.2720 (9)	0.4538 (6)	0.074 (4)*
H12B	0.1568	0.3033	0.48	0.089*
C13B	0.0418 (10)	0.2737 (9)	0.4459 (6)	0.079 (5)*
H13B	0.0133	0.3048	0.4668	0.095*
C14B	−0.0007 (10)	0.2278 (8)	0.4057 (6)	0.072 (4)*
H14B	−0.059	0.2304	0.3981	0.087*
C15B	0.0387 (8)	0.1801 (7)	0.3776 (5)	0.050 (3)*
H15B	0.0073	0.1483	0.352	0.061*
C16B	0.2781 (7)	0.1506 (6)	0.3506 (4)	0.038 (3)*
C17B	0.3488 (7)	0.1083 (7)	0.3673 (4)	0.043 (3)*
H17B	0.3434	0.0583	0.379	0.052*
C18B	0.4279 (8)	0.1373 (7)	0.3674 (5)	0.055 (4)*
H18B	0.4754	0.108	0.3797	0.066*
C19B	0.4346 (9)	0.2082 (8)	0.3497 (5)	0.065 (4)*
H19B	0.4878	0.2283	0.3493	0.077*
C20B	0.3668 (10)	0.2522 (9)	0.3322 (6)	0.079 (5)*
H20B	0.3735	0.3017	0.3198	0.095*
C21B	0.2858 (8)	0.2229 (8)	0.3328 (5)	0.058 (4)*
H21B	0.2384	0.2528	0.3211	0.069*
C22B	0.1763 (7)	−0.1613 (6)	0.3137 (4)	0.033 (3)*
C23B	0.0962 (7)	−0.1813 (7)	0.3165 (4)	0.042 (3)*
H23B	0.0561	−0.1435	0.318	0.05*
C24B	0.0745 (8)	−0.2563 (7)	0.3170 (5)	0.049 (3)*
H24B	0.02	−0.2695	0.3206	0.058*
C25B	0.1298 (8)	−0.3115 (7)	0.3126 (5)	0.052 (3)*
H25B	0.1137	−0.3627	0.3115	0.062*
C26B	0.2099 (8)	−0.2917 (8)	0.3096 (5)	0.057 (4)*
H26B	0.2495	−0.3297	0.3075	0.069*
C27B	0.2328 (8)	−0.2176 (7)	0.3097 (5)	0.051 (3)*
H27B	0.2878	−0.2048	0.3071	0.062*
C28B	0.3106 (7)	−0.0659 (6)	0.3048 (5)	0.041 (3)*
C29B	0.3719 (7)	−0.0824 (6)	0.3472 (5)	0.045 (3)*
H29B	0.3583	−0.089	0.3815	0.054*
C30B	0.4536 (8)	−0.0893 (7)	0.3401 (5)	0.052 (3)*
H30B	0.4949	−0.1015	0.3695	0.062*
C31B	0.4747 (10)	−0.0786 (9)	0.2911 (6)	0.079 (5)*
H31B	0.5306	−0.0822	0.2868	0.095*
C32B	0.4142 (10)	−0.0624 (9)	0.2477 (7)	0.080 (5)*
H32B	0.4283	−0.0558	0.2135	0.096*
C33B	0.3323 (9)	−0.0559 (8)	0.2549 (6)	0.066 (4)*
H33B	0.2909	−0.0446	0.2253	0.079*
N1S	0.5620 (11)	−0.1572 (10)	0.2003 (8)	0.121 (6)*
C1S	0.547 (2)	−0.123 (2)	0.1594 (18)	0.238 (17)*
C2S	0.5475 (19)	−0.0836 (18)	0.1067 (14)	0.194 (12)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni	0.0276 (8)	0.0323 (8)	0.0247 (7)	0.0040 (6)	0.0033 (6)	−0.0016 (6)
Fe	0.0294 (9)	0.0422 (10)	0.0244 (8)	0.0030 (8)	0.0021 (7)	−0.0021 (7)
Cl	0.0296 (15)	0.0527 (18)	0.0446 (17)	0.0089 (14)	0.0017 (13)	−0.0055 (15)
S1	0.0287 (15)	0.0346 (16)	0.0289 (14)	0.0049 (13)	0.0059 (12)	0.0022 (13)
S2	0.0360 (16)	0.0339 (16)	0.0223 (13)	0.0039 (13)	0.0043 (12)	−0.0001 (12)
S3	0.052 (2)	0.089 (3)	0.051 (2)	0.020 (2)	0.0044 (17)	−0.006 (2)
P1	0.0260 (16)	0.0344 (16)	0.0359 (16)	0.0038 (13)	0.0067 (13)	−0.0027 (14)
P2	0.0347 (17)	0.0409 (17)	0.0232 (14)	0.0095 (14)	−0.0009 (12)	−0.0007 (13)
Ni1B	0.0294 (8)	0.0333 (8)	0.0263 (7)	−0.0062 (6)	0.0027 (6)	0.0042 (7)
Fe1B	0.0234 (8)	0.0363 (9)	0.0262 (8)	0.0000 (7)	0.0022 (6)	0.0003 (7)
Cl1B	0.0315 (15)	0.0387 (16)	0.0404 (16)	−0.0083 (13)	0.0011 (12)	0.0050 (13)
S1B	0.0286 (15)	0.0301 (15)	0.0356 (15)	−0.0030 (12)	0.0019 (12)	−0.0008 (13)
S2B	0.0270 (15)	0.0347 (16)	0.0298 (14)	−0.0029 (12)	0.0045 (12)	0.0019 (13)
S3B	0.0301 (16)	0.0417 (17)	0.0314 (15)	0.0026 (13)	0.0041 (12)	0.0047 (13)
P1B	0.0329 (17)	0.0371 (17)	0.0352 (16)	−0.0084 (14)	−0.0033 (13)	0.0086 (14)
P2B	0.0328 (17)	0.0446 (19)	0.0280 (15)	−0.0103 (14)	0.0031 (13)	0.0022 (14)

Geometric parameters (Å, º)

Ni—S1	2.248 (3)	Ni1B—S2B	2.259 (3)
Ni—S2	2.243 (3)	Ni1B—P1B	2.193 (3)
Ni—P1	2.205 (3)	Ni1B—P2B	2.203 (3)
Ni—P2	2.201 (3)	Ni1B—Cl1B	2.560 (3)
Ni—Cl	2.607 (3)	Fe1B—S1B	2.290 (3)
Fe—N1	2.039 (9)	Fe1B—S2B	2.293 (3)
Fe—N2	1.991 (12)	Fe1B—S3B	2.224 (3)
Fe—N3	1.760 (12)	Fe1B—N1B	2.052 (9)
Fe—S1	2.305 (3)	Fe1B—N2B	1.794 (12)
Fe—S2	2.284 (3)	Fe1B—N3B	1.781 (12)
Fe—S3	2.222 (5)	S1B—C2B	1.845 (11)
S1—C2	1.828 (11)	S2B—C4B	1.821 (11)
S2—C4	1.814 (11)	S3B—O2B	1.457 (8)
S3—O2	1.458 (11)	S3B—O1B	1.465 (8)
S3—O1	1.460 (12)	S3B—C6B	1.839 (12)
S3—C6	1.851 (14)	P1B—C10B	1.809 (12)
P1—C16	1.812 (11)	P1B—C7B	1.817 (12)
P1—C7	1.818 (11)	P1B—C16B	1.825 (12)
P1—C10	1.833 (11)	P2B—C9B	1.811 (12)
P2—C28	1.806 (11)	P2B—C28B	1.822 (12)
P2—C9	1.830 (11)	P2B—C22B	1.843 (11)
P2—C22	1.835 (11)	N2B—O3B	1.157 (12)
N2—O3	1.023 (16)	N3B—O4B	1.157 (12)
N3—O4	1.178 (12)	N1B—C1B	1.500 (13)
N1—C3	1.469 (15)	N1B—C5B	1.510 (13)
N1—C5	1.489 (14)	N1B—C3B	1.528 (13)

N1—C1	1.517 (17)	C1B—C2B	1.516 (14)
C1—C2	1.488 (18)	C1B—H1B1	0.9900
C1—H1A	0.9900	C1B—H1B2	0.9900
C1—H1B	0.9900	C2B—H2B1	0.9900
C2—H2A	0.9900	C2B—H2B2	0.9900
C2—H2B	0.9900	C3B—C4B	1.498 (14)
C3—C4	1.457 (17)	C3B—H3B1	0.9900
C3—H3A	0.9900	C3B—H3B2	0.9900
C3—H3B	0.9900	C4B—H4B1	0.9900
C4—H4A	0.9900	C4B—H4B2	0.9900
C4—H4B	0.9900	C5B—C6B	1.512 (15)
C5—C6	1.584 (18)	C5B—H5B1	0.9900
C5—H5A	0.9900	C5B—H5B2	0.9900
C5—H5B	0.9900	C6B—H6B1	0.9900
C6—H6A	0.9900	C6B—H6B2	0.9900
C6—H6B	0.9900	C7B—C8B	1.549 (16)
C7—C8	1.554 (16)	C7B—H7B1	0.9900
C7—H7A	0.9900	C7B—H7B2	0.9900
C7—H7B	0.9900	C8B—C9B	1.521 (16)
C8—C9	1.527 (15)	C8B—H8B1	0.9900
C8—H8A	0.9900	C8B—H8B2	0.9900
C8—H8B	0.9900	C9B—H9B1	0.9900
C9—H9A	0.9900	C9B—H9B2	0.9900
C9—H9B	0.9900	C10B—C11B	1.389 (16)
C10—C11	1.376 (14)	C10B—C15B	1.414 (16)
C10—C15	1.397 (15)	C11B—C12B	1.394 (19)
C11—C12	1.389 (16)	C11B—H11B	0.9500
C11—H11	0.9500	C12B—C13B	1.37 (2)
C12—C13	1.391 (16)	C12B—H12B	0.9500
C12—H12	0.9500	C13B—C14B	1.40 (2)
C13—C14	1.380 (16)	C13B—H13B	0.9500
C13—H13	0.9500	C14B—C15B	1.351 (18)
C14—C15	1.401 (16)	C14B—H14B	0.9500
C14—H14	0.9500	C15B—H15B	0.9500
C15—H15	0.9500	C16B—C21B	1.380 (17)
C16—C17	1.391 (15)	C16B—C17B	1.393 (15)
C16—C21	1.396 (15)	C17B—C18B	1.402 (16)
C17—C18	1.391 (16)	C17B—H17B	0.9500
C17—H17	0.9500	C18B—C19B	1.353 (18)
C18—C19	1.379 (17)	C18B—H18B	0.9500
C18—H18	0.9500	C19B—C20B	1.378 (19)
C19—C20	1.342 (16)	C19B—H19B	0.9500
C19—H19	0.9500	C20B—C21B	1.439 (19)
C20—C21	1.387 (16)	C20B—H20B	0.9500
C20—H20	0.9500	C21B—H21B	0.9500
C21—H21	0.9500	C22B—C23B	1.384 (15)
C22—C27	1.353 (15)	C22B—C27B	1.385 (16)
C22—C23	1.418 (16)	C23B—C24B	1.383 (16)

C23—C24	1.397 (17)	C23B—H23B	0.9500
C23—H23	0.9500	C24B—C25B	1.360 (16)
C24—C25	1.303 (17)	C24B—H24B	0.9500
C24—H24	0.9500	C25B—C26B	1.384 (17)
C25—C26	1.408 (18)	C25B—H25B	0.9500
C25—H25	0.9500	C26B—C27B	1.372 (17)
C26—C27	1.404 (17)	C26B—H26B	0.9500
C26—H26	0.9500	C27B—H27B	0.9500
C27—H27	0.9500	C28B—C29B	1.379 (15)
C28—C29	1.377 (15)	C28B—C33B	1.397 (17)
C28—C33	1.395 (15)	C29B—C30B	1.399 (16)
C29—C30	1.420 (18)	C29B—H29B	0.9500
C29—H29	0.9500	C30B—C31B	1.371 (19)
C30—C31	1.383 (17)	C30B—H30B	0.9500
C30—H30	0.9500	C31B—C32B	1.39 (2)
C31—C32	1.350 (16)	C31B—H31B	0.9500
C31—H31	0.9500	C32B—C33B	1.40 (2)
C32—C33	1.368 (16)	C32B—H32B	0.9500
C32—H32	0.9500	C33B—H33B	0.9500
C33—H33	0.9500	N1S—C1S	1.19 (4)
Ni1B—S1B	2.253 (3)	C1S—C2S	1.53 (4)

P2—Ni—P1	92.40 (12)	P1B—Ni1B—S1B	86.56 (12)
P2—Ni—S2	88.81 (11)	P2B—Ni1B—S1B	158.60 (12)
P1—Ni—S2	163.84 (12)	P1B—Ni1B—S2B	166.29 (12)
P2—Ni—S1	164.48 (12)	P2B—Ni1B—S2B	90.07 (12)
P1—Ni—S1	89.66 (11)	S1B—Ni1B—S2B	85.77 (11)
S2—Ni—S1	85.03 (10)	P1B—Ni1B—Cl1B	88.41 (11)
P2—Ni—Cl	89.02 (11)	P2B—Ni1B—Cl1B	94.63 (11)
P1—Ni—Cl	89.14 (11)	S1B—Ni1B—Cl1B	106.73 (11)
S2—Ni—Cl	107.00 (11)	S2B—Ni1B—Cl1B	104.68 (10)
S1—Ni—Cl	106.39 (11)	N3B—Fe1B—N2B	90.3 (5)
N3—Fe—N2	96.7 (5)	N3B—Fe1B—N1B	175.0 (4)
N3—Fe—N1	178.3 (5)	N2B—Fe1B—N1B	94.6 (4)
N2—Fe—N1	84.9 (4)	N3B—Fe1B—S3B	93.3 (4)
N3—Fe—S3	91.9 (4)	N2B—Fe1B—S3B	90.0 (4)
N2—Fe—S3	87.9 (3)	N1B—Fe1B—S3B	87.4 (3)
N1—Fe—S3	88.4 (3)	N3B—Fe1B—S1B	93.6 (4)
N3—Fe—S2	90.2 (4)	N2B—Fe1B—S1B	93.0 (4)
N2—Fe—S2	172.9 (3)	N1B—Fe1B—S1B	85.4 (2)
N1—Fe—S2	88.1 (3)	S3B—Fe1B—S1B	172.44 (12)
S3—Fe—S2	93.53 (13)	N3B—Fe1B—S2B	86.9 (4)
N3—Fe—S1	93.5 (4)	N2B—Fe1B—S2B	175.8 (4)
N2—Fe—S1	95.1 (3)	N1B—Fe1B—S2B	88.1 (2)
N1—Fe—S1	86.0 (3)	S3B—Fe1B—S2B	93.28 (11)
S3—Fe—S1	173.46 (14)	S1B—Fe1B—S2B	84.11 (11)
S2—Fe—S1	82.78 (11)	C2B—S1B—Ni1B	108.2 (4)
C2—S1—Ni	107.8 (4)	C2B—S1B—Fe1B	100.1 (4)

C2—S1—Fe	99.6 (4)	Ni1B—S1B—Fe1B	94.75 (11)
Ni—S1—Fe	95.55 (11)	C4B—S2B—Ni1B	109.6 (4)
C4—S2—Ni	108.4 (4)	C4B—S2B—Fe1B	97.3 (4)
C4—S2—Fe	97.0 (4)	Ni1B—S2B—Fe1B	94.52 (11)
Ni—S2—Fe	96.27 (12)	O2B—S3B—O1B	114.7 (4)
O2—S3—O1	113.9 (7)	O2B—S3B—C6B	105.9 (5)
O2—S3—C6	105.4 (7)	O1B—S3B—C6B	105.0 (5)
O1—S3—C6	105.7 (7)	O2B—S3B—Fe1B	116.6 (3)
O2—S3—Fe	118.1 (5)	O1B—S3B—Fe1B	111.9 (3)
O1—S3—Fe	112.8 (5)	C6B—S3B—Fe1B	100.8 (4)
C6—S3—Fe	98.6 (5)	C10B—P1B—C7B	103.2 (5)
C16—P1—C7	104.6 (5)	C10B—P1B—C16B	103.3 (5)
C16—P1—C10	103.7 (5)	C7B—P1B—C16B	105.6 (6)
C7—P1—C10	103.0 (5)	C10B—P1B—Ni1B	113.8 (4)
C16—P1—Ni	113.5 (4)	C7B—P1B—Ni1B	116.2 (4)
C7—P1—Ni	117.1 (4)	C16B—P1B—Ni1B	113.4 (4)
C10—P1—Ni	113.5 (4)	C9B—P2B—C28B	107.1 (6)
C28—P2—C9	104.6 (5)	C9B—P2B—C22B	102.1 (5)
C28—P2—C22	103.2 (5)	C28B—P2B—C22B	101.3 (5)
C9—P2—C22	104.0 (5)	C9B—P2B—Ni1B	114.7 (4)
C28—P2—Ni	114.8 (4)	C28B—P2B—Ni1B	115.7 (4)
C9—P2—Ni	115.4 (4)	C22B—P2B—Ni1B	114.4 (4)
C22—P2—Ni	113.5 (4)	C1B—N1B—C5B	107.2 (8)
C3—N1—C5	109.4 (9)	C1B—N1B—C3B	108.2 (8)
C3—N1—C1	111.7 (10)	C5B—N1B—C3B	109.6 (8)
C5—N1—C1	104.8 (9)	C1B—N1B—Fe1B	108.7 (6)
C3—N1—Fe	113.5 (8)	C5B—N1B—Fe1B	109.1 (6)
C5—N1—Fe	109.2 (7)	C3B—N1B—Fe1B	113.9 (6)
C1—N1—Fe	107.8 (8)	O3B—N2B—Fe1B	176.3 (10)
O3—N2—Fe	149.3 (14)	O4B—N3B—Fe1B	177.2 (10)
O4—N3—Fe	175.1 (10)	N1B—C1B—C2B	112.3 (9)
C2—C1—N1	115.0 (12)	N1B—C1B—H1B1	109.1
C2—C1—H1A	108.5	C2B—C1B—H1B1	109.1
N1—C1—H1A	108.5	N1B—C1B—H1B2	109.1
C2—C1—H1B	108.5	C2B—C1B—H1B2	109.1
N1—C1—H1B	108.5	H1B1—C1B—H1B2	107.9
H1A—C1—H1B	107.5	C1B—C2B—S1B	110.0 (7)
C1—C2—S1	111.0 (9)	C1B—C2B—H2B1	109.7
C1—C2—H2A	109.4	S1B—C2B—H2B1	109.7
S1—C2—H2A	109.4	C1B—C2B—H2B2	109.7
C1—C2—H2B	109.4	S1B—C2B—H2B2	109.7
S1—C2—H2B	109.4	H2B1—C2B—H2B2	108.2
H2A—C2—H2B	108.0	C4B—C3B—N1B	114.3 (9)
C4—C3—N1	119.3 (11)	C4B—C3B—H3B1	108.7
C4—C3—H3A	107.5	N1B—C3B—H3B1	108.7
N1—C3—H3A	107.5	C4B—C3B—H3B2	108.7
C4—C3—H3B	107.5	N1B—C3B—H3B2	108.7
N1—C3—H3B	107.5	H3B1—C3B—H3B2	107.6

H3A—C3—H3B	107.0	C3B—C4B—S2B	111.2 (8)
C3—C4—S2	112.1 (9)	C3B—C4B—H4B1	109.4
C3—C4—H4A	109.2	S2B—C4B—H4B1	109.4
S2—C4—H4A	109.2	C3B—C4B—H4B2	109.4
C3—C4—H4B	109.2	S2B—C4B—H4B2	109.4
S2—C4—H4B	109.2	H4B1—C4B—H4B2	108.0
H4A—C4—H4B	107.9	N1B—C5B—C6B	110.8 (9)
N1—C5—C6	105.9 (10)	N1B—C5B—H5B1	109.5
N1—C5—H5A	110.6	C6B—C5B—H5B1	109.5
C6—C5—H5A	110.6	N1B—C5B—H5B2	109.5
N1—C5—H5B	110.6	C6B—C5B—H5B2	109.5
C6—C5—H5B	110.6	H5B1—C5B—H5B2	108.1
H5A—C5—H5B	108.7	C5B—C6B—S3B	107.9 (8)
C5—C6—S3	108.9 (9)	C5B—C6B—H6B1	110.1
C5—C6—H6A	109.9	S3B—C6B—H6B1	110.1
S3—C6—H6A	109.9	C5B—C6B—H6B2	110.1
C5—C6—H6B	109.9	S3B—C6B—H6B2	110.1
S3—C6—H6B	109.9	H6B1—C6B—H6B2	108.4
H6A—C6—H6B	108.3	C8B—C7B—P1B	114.3 (8)
C8—C7—P1	114.1 (8)	C8B—C7B—H7B1	108.7
C8—C7—H7A	108.7	P1B—C7B—H7B1	108.7
P1—C7—H7A	108.7	C8B—C7B—H7B2	108.7
C8—C7—H7B	108.7	P1B—C7B—H7B2	108.7
P1—C7—H7B	108.7	H7B1—C7B—H7B2	107.6
H7A—C7—H7B	107.6	C9B—C8B—C7B	112.9 (10)
C9—C8—C7	112.6 (10)	C9B—C8B—H8B1	109.0
C9—C8—H8A	109.1	C7B—C8B—H8B1	109.0
C7—C8—H8A	109.1	C9B—C8B—H8B2	109.0
C9—C8—H8B	109.1	C7B—C8B—H8B2	109.0
C7—C8—H8B	109.1	H8B1—C8B—H8B2	107.8
H8A—C8—H8B	107.8	C8B—C9B—P2B	114.7 (8)
C8—C9—P2	113.1 (8)	C8B—C9B—H9B1	108.6
C8—C9—H9A	109.0	P2B—C9B—H9B1	108.6
P2—C9—H9A	109.0	C8B—C9B—H9B2	108.6
C8—C9—H9B	109.0	P2B—C9B—H9B2	108.6
P2—C9—H9B	109.0	H9B1—C9B—H9B2	107.6
H9A—C9—H9B	107.8	C11B—C10B—C15B	115.5 (11)
C11—C10—C15	119.8 (11)	C11B—C10B—P1B	122.5 (9)
C11—C10—P1	121.0 (9)	C15B—C10B—P1B	121.7 (9)
C15—C10—P1	119.1 (8)	C10B—C11B—C12B	122.8 (13)
C10—C11—C12	120.1 (11)	C10B—C11B—H11B	118.6
C10—C11—H11	119.9	C12B—C11B—H11B	118.6
C12—C11—H11	119.9	C13B—C12B—C11B	120.3 (15)
C11—C12—C13	121.2 (12)	C13B—C12B—H12B	119.9
C11—C12—H12	119.4	C11B—C12B—H12B	119.9
C13—C12—H12	119.4	C12B—C13B—C14B	117.5 (16)
C14—C13—C12	118.2 (12)	C12B—C13B—H13B	121.2
C14—C13—H13	120.9	C14B—C13B—H13B	121.2

C12—C13—H13	120.9	C15B—C14B—C13B	122.2 (15)
C13—C14—C15	121.4 (12)	C15B—C14B—H14B	118.9
C13—C14—H14	119.3	C13B—C14B—H14B	118.9
C15—C14—H14	119.3	C14B—C15B—C10B	121.6 (13)
C10—C15—C14	119.1 (11)	C14B—C15B—H15B	119.2
C10—C15—H15	120.4	C10B—C15B—H15B	119.2
C14—C15—H15	120.4	C21B—C16B—C17B	119.1 (11)
C17—C16—C21	116.3 (11)	C21B—C16B—P1B	122.3 (9)
C17—C16—P1	120.2 (9)	C17B—C16B—P1B	118.6 (9)
C21—C16—P1	123.5 (8)	C16B—C17B—C18B	122.2 (12)
C18—C17—C16	122.8 (12)	C16B—C17B—H17B	118.9
C18—C17—H17	118.6	C18B—C17B—H17B	118.9
C16—C17—H17	118.6	C19B—C18B—C17B	118.3 (13)
C19—C18—C17	118.4 (12)	C19B—C18B—H18B	120.9
C19—C18—H18	120.8	C17B—C18B—H18B	120.9
C17—C18—H18	120.8	C18B—C19B—C20B	122.0 (15)
C20—C19—C18	120.3 (13)	C18B—C19B—H19B	119.0
C20—C19—H19	119.9	C20B—C19B—H19B	119.0
C18—C19—H19	119.9	C19B—C20B—C21B	119.7 (15)
C19—C20—C21	121.5 (13)	C19B—C20B—H20B	120.1
C19—C20—H20	119.2	C21B—C20B—H20B	120.1
C21—C20—H20	119.2	C16B—C21B—C20B	118.7 (13)
C20—C21—C16	120.7 (11)	C16B—C21B—H21B	120.6
C20—C21—H21	119.7	C20B—C21B—H21B	120.6
C16—C21—H21	119.7	C23B—C22B—C27B	118.6 (11)
C27—C22—C23	120.7 (11)	C23B—C22B—P2B	119.3 (9)
C27—C22—P2	120.2 (9)	C27B—C22B—P2B	122.1 (9)
C23—C22—P2	118.9 (9)	C22B—C23B—C24B	120.1 (11)
C24—C23—C22	117.5 (12)	C22B—C23B—H23B	119.9
C24—C23—H23	121.2	C24B—C23B—H23B	119.9
C22—C23—H23	121.2	C25B—C24B—C23B	121.2 (12)
C25—C24—C23	121.2 (14)	C25B—C24B—H24B	119.4
C25—C24—H24	119.4	C23B—C24B—H24B	119.4
C23—C24—H24	119.4	C24B—C25B—C26B	118.8 (13)
C24—C25—C26	123.1 (15)	C24B—C25B—H25B	120.6
C24—C25—H25	118.5	C26B—C25B—H25B	120.6
C26—C25—H25	118.5	C27B—C26B—C25B	120.7 (13)
C27—C26—C25	116.7 (13)	C27B—C26B—H26B	119.6
C27—C26—H26	121.7	C25B—C26B—H26B	119.6
C25—C26—H26	121.7	C26B—C27B—C22B	120.5 (13)
C22—C27—C26	120.8 (12)	C26B—C27B—H27B	119.7
C22—C27—H27	119.6	C22B—C27B—H27B	119.7
C26—C27—H27	119.6	C29B—C28B—C33B	118.5 (12)
C29—C28—C33	117.8 (11)	C29B—C28B—P2B	118.4 (9)
C29—C28—P2	119.4 (9)	C33B—C28B—P2B	123.0 (10)
C33—C28—P2	122.9 (8)	C28B—C29B—C30B	120.8 (12)
C28—C29—C30	119.8 (12)	C28B—C29B—H29B	119.6
C28—C29—H29	120.1	C30B—C29B—H29B	119.6

C30—C29—H29	120.1	C31B—C30B—C29B	120.5 (13)
C31—C30—C29	119.9 (13)	C31B—C30B—H30B	119.7
C31—C30—H30	120.1	C29B—C30B—H30B	119.7
C29—C30—H30	120.1	C30B—C31B—C32B	120.0 (16)
C32—C31—C30	119.9 (13)	C30B—C31B—H31B	120.0
C32—C31—H31	120.1	C32B—C31B—H31B	120.0
C30—C31—H31	120.1	C31B—C32B—C33B	119.4 (16)
C31—C32—C33	120.5 (13)	C31B—C32B—H32B	120.3
C31—C32—H32	119.8	C33B—C32B—H32B	120.3
C33—C32—H32	119.8	C28B—C33B—C32B	120.8 (14)
C32—C33—C28	122.2 (11)	C28B—C33B—H33B	119.6
C32—C33—H33	118.9	C32B—C33B—H33B	119.6
C28—C33—H33	118.9	N1S—C1S—C2S	168 (4)
P1B—Ni1B—P2B	92.95 (12)		

Fe—S1—C2—C1	6.3 (9)	Fe1B—S1B—C2B—C1B	10.1 (8)
S1—C2—C1—N1	−37.0 (14)	S1B—C2B—C1B—N1B	−41.4 (10)
C2—C1—N1—Fe	52.0 (13)	C2B—C1B—N1B—Fe1B	55.4 (9)
Fe—S2—C4—C3	31.3 (9)	Fe1B—S2B—C4B—C3B	36.7 (7)
S2—C4—C3—N1	−33.9 (14)	S2B—C4B—C3B—N1B	−43.8 (11)
C4—C3—N1—Fe	15.8 (14)	C4B—C3B—N1B—Fe1B	26.4 (11)
Fe—S3—C6—C5	−25.3 (9)	Fe1B—S3B—C6B—C5B	−24.8 (8)
S3—C6—C5—N1	53.5 (11)	S3B—C6B—C5B—N1B	50.6 (10)
C6—C5—N1—Fe	−57.2 (10)	C6B—C5B—N1B—Fe1B	−53.0 (9)
Ni—P1—C7—C8	−54.9 (9)	Ni1B—P1B—C7B—C8B	−55.9 (10)
P1—C7—C8—C9	69.6 (11)	P1B—C7B—C8B—C9B	68.7 (12)
C7—C8—C9—P2	−72.8 (11)	C7B—C8B—C9B—P2B	−71.4 (12)
C8—C9—P2—Ni	60.9 (8)	C8B—C9B—P2B—Ni1B	59.8 (10)