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Chlorido(ethyldiphenylphosphine- κP)-(1-pyrrolidinecarbodithioato- $\kappa^2 S, S'$)-nickel(II)

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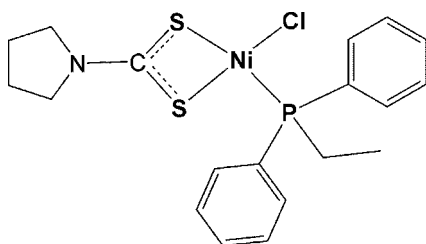
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Key indicators: single-crystal X-ray study; $T = 299$ K; mean $\sigma(C-C) = 0.006$ Å; R factor = 0.040; wR factor = 0.114; data-to-parameter ratio = 16.1.

In the crystal structure of the title complex, $[Ni(C_5H_8NS_2)Cl(C_{14}H_{15}P)]$, the Ni atom is coordinated by an S, S' -chelating dithiocarbamate, a chloride and a diphenylethylphosphine ligand in a distorted square-planar arrangement.

Related literature

For related literature, see: Allen (2002); Darkwa *et al.* (1999); Kropidłowska, Chojnacki *et al.* (2007); Kropidłowska, Janczak *et al.* (2007); Pastorek *et al.* (1996, 1999); Reger & Collins (1995).



Experimental

Crystal data

$[Ni(C_5H_8NS_2)Cl(C_{14}H_{15}P)]$
 $M_r = 454.63$

Monoclinic, $P2_1/c$
 $a = 6.5218$ (5) Å

$b = 19.1695$ (15) Å
 $c = 16.6178$ (14) Å
 $\beta = 90.786$ (6)°
 $V = 2077.4$ (3) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 1.34$ mm⁻¹
 $T = 299$ (2) K
 $0.50 \times 0.21 \times 0.17$ mm

Data collection

Kuma KM-4-CCD diffractometer
Absorption correction: refined from
 ΔF (Walker & Stuart, 1983)
 $T_{min} = 0.553$, $T_{max} = 0.804$

10912 measured reflections
3637 independent reflections
2989 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.042$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.113$
 $S = 1.08$
3637 reflections

226 parameters
H-atom parameters constrained
 $\Delta\rho_{max} = 0.57$ e Å⁻³
 $\Delta\rho_{min} = -0.35$ e Å⁻³

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2003); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

The authors acknowledge Professor J. Pikies for his donation of the sample of $NiCl_2(PPh_2Et)_2$ and J. Gołaszewska for her help during the crystallization. This work was supported by the Ministry of Science and Higher Education (Poland), grant No. 1 T09A 117 30. A. Kropidłowska thanks the Foundation for Polish Science for a fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2563).

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Chlorido(ethyldiphenylphosphine- κP)(1-pyrrolidinecarbodithioato- $\kappa^2 S, S'$)nickel(II)

Anna Kropidłowska, Ilona Turowska-Tyrk and Barbara Becker

S1. Comment

Metal (Ni, Pd) complexes in which the atom is coordinated by a *S,S*-chelating dithiocarbamate, one halogenide and one phosphine have been investigated and used to obtain compounds with a sulfur rich kernel arising from the presence of two different *S*-donor ligands (Darkwa *et al.*, 1999; Pastorek *et al.*, 1999; Reger & Collins, 1995). Several structures of such species are stored in the Cambridge Structural Database (CSD-2007, Allen 2002).

Recently, we reported the synthesis of $[\text{Ni}\{\text{S}_2\text{CN}(\text{CH}_2)_4\}(\text{Cl})(\text{PPh}_3)]$ (Kropidłowska, Janczak *et al.*, 2007) solvated by a chloroform molecule, which interacts with the complex by a weak C—H \cdots S hydrogen bond. The structure of homologous hemisolvated $[\text{Ni}\{\text{S}_2\text{CN}(\text{CH}_2)_4\}(\text{Br})(\text{PPh}_3)]$ has also been reported (Pastorek *et al.*, 1996). In the present paper we describe the structure of another nickel(II) complex - (1-pyrrolidinylcarbodithioato-*S,S'*) -chlorido-(diphenylethylphosphine)nickel(II), $[\text{Ni}\{\text{S}_2\text{CN}(\text{CH}_2)_4\}(\text{Cl})(\text{PPh}_2\text{Et})]$ (I) obtained by essentially quantitative metathesis of *trans*-dichlorobis(diphenylethylphosphine)-nickel(II) and bis(1-pyrrolidinylcarbodithioato-*S,S'*)nickel(II). The molecular structure of (I) with the atom numbering scheme is shown in Figure 1.

In this compound the metal(II) ion is four-coordinated within a typical square planar $[\text{NiClS}_2\text{P}]$ heterogeneous coordination sphere. The dithiocarbamate ligand acts as a bidentate chelate, coordinating to Ni *via* both S atoms and thus introducing a deformation of the coordination geometry. Atom S1 is located *trans* to the Cl ligand and atom S2 is *trans* to the diphenylethylphosphine ligand. Although (I) was obtained in the same manner as previously mentioned $[\text{Ni}\{\text{S}_2\text{CN}(\text{CH}_2)_4\}(\text{Cl})(\text{PPh}_3)]$ it did not retain the solvent within its crystal structure, similarly to previously described $[\text{Ni}\{\text{S}_2\text{CN}(\text{C}_4\text{H}_8\text{O})\}(\text{Cl})(\text{PPh}_3)]$ (Kropidłowska, Chojnacki *et al.*, 2007). The schematic drawing of the crystal packing in (I) is presented in Figure 2.

S2. Experimental

Nickel chloride, $\text{NiCl}_2 \cdot 6\text{H}_2\text{O}$ (0.594 g, 0.0025 mol, purchased from POCh) was dissolved in 50 ml of methanol/water (10/1, v/v) and this solution was added dropwise to the ammonium salt of pyrrolidinecarbodithioic acid $\text{C}_4\text{H}_8\text{NCS}_2\text{NH}_4$ (0.82 g, 0.005 mol, Fluka) dissolved in methanol/water. This mixture was stirred vigorously under argon atmosphere for ca 20 minutes, then filtered and the filtrate left for crystallization at 278 K. After a week the green crystalline product, namely $\text{Ni}(\text{S}_2\text{CNC}_4\text{H}_8)_2$ was collected. It was further dissolved (0.199 g, 0.00057 mol) in 10 ml of chloroform and mixed with solution of equimolar amount of $\text{NiCl}_2(\text{PPh}_2\text{Et})_2$ (0.315 g). The mixture which turned into deep violet colour, was stirred for 10 minutes and then filtered. To the filtrate 10 ml of Et_2O was added. After two days violet crystals were collected and washed with several portions of ether.

S3. Refinement

All H atoms were positioned geometrically and treated as riding with C—H = 0.93 - 0.97 Å, and with $U_{\text{iso}}(\text{H})$ values of $1.2 \times U_{\text{eq}}$ of the parent methylene carbon and $U_{\text{iso}}(\text{H})$ values of $1.5 \times U_{\text{eq}}$ of the methyl group carbon.

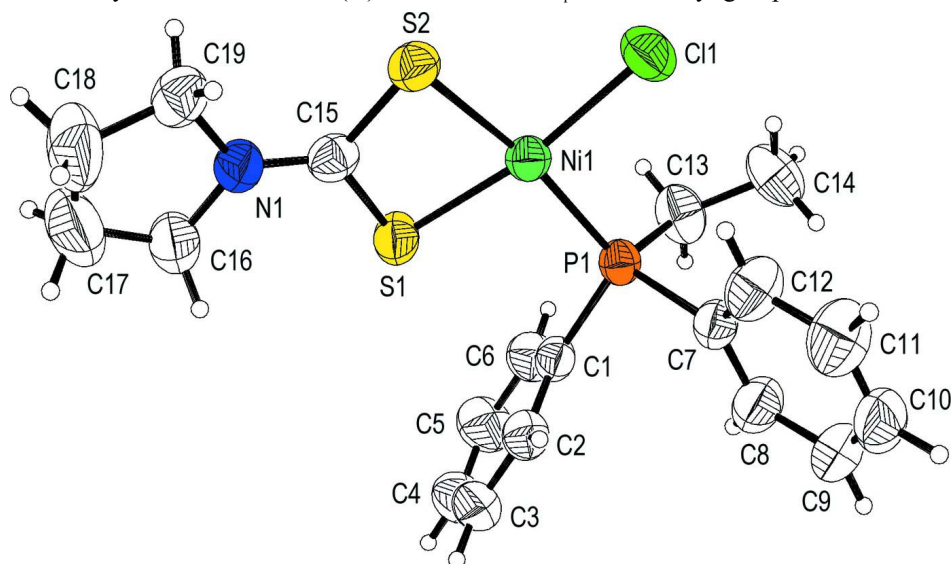
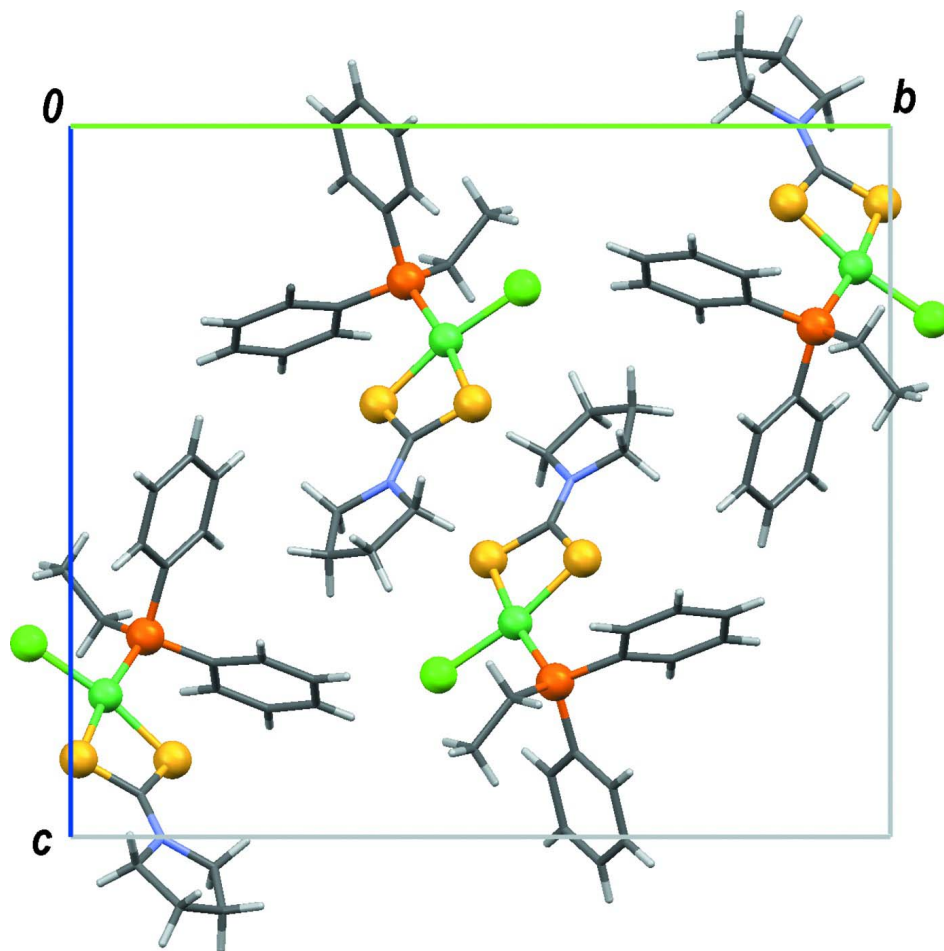


Figure 1

Molecular structure and atom-numbering scheme for the title complex (I) with displacement ellipsoids drawn at 50% probability level. H atoms are represented as circles of arbitrary size.

**Figure 2**

Schematic drawing of the crystal packing down the a axis.

Chlorido(ethyldiphenylphosphine- κP)(1-pyrrolidinecarbodithioato- $\kappa^2 S, S'$)nickel(II)

Crystal data

$[\text{Ni}(\text{C}_5\text{H}_8\text{NS}_2)\text{Cl}(\text{C}_{14}\text{H}_{15}\text{P})]$

$M_r = 454.63$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 6.5218\ (5)\ \text{\AA}$

$b = 19.1695\ (15)\ \text{\AA}$

$c = 16.6178\ (14)\ \text{\AA}$

$\beta = 90.786\ (6)^\circ$

$V = 2077.4\ (3)\ \text{\AA}^3$

$Z = 4$

$F(000) = 944$

$D_x = 1.454\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 3645 reflections

$\theta = 3.5\text{--}23.0^\circ$

$\mu = 1.34\ \text{mm}^{-1}$

$T = 299\ \text{K}$

Block, violet

$0.50 \times 0.21 \times 0.17\ \text{mm}$

Data collection

Kuma KM-4-CCD

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

ω scans

Absorption correction: part of the refinement

model (ΔF)

(Walker & Stuart, 1983)

$T_{\min} = 0.553$, $T_{\max} = 0.804$

10912 measured reflections

3637 independent reflections
 2989 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.042$
 $\theta_{\text{max}} = 25.0^\circ$, $\theta_{\text{min}} = 3.1^\circ$

$h = -6 \rightarrow 7$
 $k = -22 \rightarrow 22$
 $l = -19 \rightarrow 18$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.040$
 $wR(F^2) = 0.113$
 $S = 1.08$
 3637 reflections
 226 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
 $w = 1/[\sigma^2(F_o^2) + (0.0634P)^2 + 0.6647P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.57 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.35 \text{ e } \text{\AA}^{-3}$

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.41398 (6)	0.542285 (19)	0.69879 (2)	0.04145 (15)
Cl1	0.45930 (14)	0.44894 (4)	0.77213 (6)	0.0630 (3)
P1	0.19702 (11)	0.59106 (4)	0.78208 (5)	0.0397 (2)
S1	0.38209 (13)	0.62417 (5)	0.60835 (5)	0.0544 (2)
S2	0.64891 (13)	0.50962 (4)	0.60948 (5)	0.0508 (2)
N1	0.6761 (4)	0.61076 (14)	0.49827 (16)	0.0524 (7)
C1	0.0929 (4)	0.67350 (15)	0.74538 (17)	0.0421 (7)
C2	0.2112 (5)	0.73347 (17)	0.7499 (2)	0.0534 (8)
H2	0.3426	0.7314	0.7722	0.064*
C3	0.1353 (7)	0.79645 (19)	0.7214 (2)	0.0658 (10)
H3	0.2148	0.8366	0.7255	0.079*
C4	-0.0576 (7)	0.7995 (2)	0.6872 (3)	0.0732 (11)
H4	-0.1092	0.8418	0.6686	0.088*
C5	-0.1733 (7)	0.7405 (2)	0.6805 (3)	0.0743 (11)
H5	-0.3029	0.7426	0.6566	0.089*
C6	-0.0994 (5)	0.67784 (19)	0.7092 (2)	0.0571 (9)
H6	-0.1796	0.6379	0.7041	0.069*
C7	0.2986 (5)	0.61533 (16)	0.88112 (18)	0.0447 (7)
C8	0.1922 (6)	0.6611 (2)	0.9294 (2)	0.0651 (10)
H8	0.0725	0.6817	0.9097	0.078*
C9	0.2601 (8)	0.6766 (2)	1.0060 (2)	0.0790 (12)



H9	0.1865	0.7076	1.0376	0.095*
C10	0.4359 (8)	0.6466 (2)	1.0358 (2)	0.0769 (12)
H10	0.4819	0.6569	1.0876	0.092*
C11	0.5419 (7)	0.6020 (3)	0.9890 (3)	0.0833 (13)
H11	0.6618	0.5818	1.0090	0.100*
C12	0.4748 (5)	0.5858 (2)	0.9115 (2)	0.0637 (10)
H12	0.5495	0.5549	0.8802	0.076*
C13	-0.0307 (5)	0.53894 (19)	0.8047 (2)	0.0614 (9)
H13A	-0.1441	0.5706	0.8141	0.074*
H13B	-0.0657	0.5114	0.7575	0.074*
C14	-0.0117 (6)	0.4907 (2)	0.8755 (3)	0.0737 (11)
H14A	-0.1381	0.4659	0.8821	0.111*
H14B	0.0179	0.5174	0.9232	0.111*
H14C	0.0973	0.4581	0.8666	0.111*
C15	0.5834 (5)	0.58493 (17)	0.55992 (19)	0.0468 (7)
C16	0.6134 (7)	0.6751 (2)	0.4568 (2)	0.0740 (11)
H16A	0.4787	0.6699	0.4321	0.089*
H16B	0.6106	0.7141	0.4940	0.089*
C17	0.7689 (10)	0.6853 (3)	0.3962 (4)	0.125 (2)
H17A	0.7055	0.6832	0.3431	0.151*
H17B	0.8298	0.7312	0.4028	0.151*
C18	0.9245 (7)	0.6337 (3)	0.4024 (3)	0.1021 (17)
H18A	1.0527	0.6550	0.4198	0.123*
H18B	0.9453	0.6122	0.3503	0.123*
C19	0.8606 (5)	0.5801 (2)	0.4617 (2)	0.0609 (9)
H19A	0.8285	0.5362	0.4353	0.073*
H19B	0.9673	0.5722	0.5020	0.073*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0434 (2)	0.0415 (2)	0.0394 (2)	0.00158 (16)	-0.00237 (16)	-0.00039 (16)
Cl1	0.0697 (6)	0.0521 (5)	0.0672 (6)	0.0089 (4)	0.0010 (4)	0.0144 (4)
P1	0.0380 (4)	0.0437 (4)	0.0373 (4)	-0.0021 (3)	-0.0015 (3)	0.0024 (3)
S1	0.0597 (5)	0.0577 (5)	0.0459 (5)	0.0158 (4)	0.0092 (4)	0.0086 (4)
S2	0.0543 (5)	0.0506 (5)	0.0475 (5)	0.0093 (4)	0.0022 (4)	-0.0024 (4)
N1	0.0547 (16)	0.0542 (16)	0.0486 (15)	0.0051 (13)	0.0081 (13)	0.0023 (13)
C1	0.0450 (16)	0.0463 (17)	0.0351 (15)	0.0027 (13)	0.0054 (12)	0.0009 (13)
C2	0.0593 (19)	0.0530 (19)	0.0481 (18)	-0.0062 (16)	0.0068 (15)	0.0000 (15)
C3	0.085 (3)	0.050 (2)	0.063 (2)	-0.0068 (19)	0.019 (2)	0.0035 (17)
C4	0.091 (3)	0.054 (2)	0.074 (3)	0.022 (2)	0.010 (2)	0.0109 (19)
C5	0.073 (2)	0.067 (3)	0.082 (3)	0.018 (2)	-0.008 (2)	0.013 (2)
C6	0.056 (2)	0.057 (2)	0.058 (2)	0.0034 (16)	-0.0081 (16)	0.0028 (16)
C7	0.0473 (17)	0.0488 (17)	0.0381 (16)	-0.0055 (13)	-0.0004 (13)	0.0008 (13)
C8	0.077 (2)	0.070 (2)	0.048 (2)	0.0109 (19)	-0.0018 (17)	-0.0049 (18)
C9	0.116 (4)	0.074 (3)	0.047 (2)	0.000 (3)	0.008 (2)	-0.008 (2)
C10	0.105 (3)	0.078 (3)	0.048 (2)	-0.025 (3)	-0.014 (2)	0.001 (2)
C11	0.074 (3)	0.111 (4)	0.064 (3)	0.001 (2)	-0.029 (2)	-0.002 (3)

C12	0.0516 (19)	0.086 (3)	0.054 (2)	0.0034 (18)	-0.0077 (16)	-0.0089 (19)
C13	0.0479 (19)	0.070 (2)	0.066 (2)	-0.0158 (16)	-0.0042 (16)	0.0143 (18)
C14	0.061 (2)	0.066 (2)	0.094 (3)	-0.0119 (18)	0.002 (2)	0.027 (2)
C15	0.0475 (17)	0.0486 (18)	0.0443 (17)	0.0054 (14)	-0.0042 (13)	-0.0050 (14)
C16	0.090 (3)	0.069 (2)	0.064 (2)	0.011 (2)	0.020 (2)	0.015 (2)
C17	0.145 (5)	0.091 (4)	0.142 (5)	0.014 (4)	0.076 (4)	0.045 (4)
C18	0.081 (3)	0.127 (4)	0.100 (4)	0.016 (3)	0.043 (3)	0.042 (3)
C19	0.0510 (19)	0.070 (2)	0.062 (2)	-0.0008 (17)	0.0124 (16)	-0.0050 (18)

Geometric parameters (Å, °)

Ni1—S1	2.1812 (9)	C8—H8	0.9300
Ni1—C11	2.1828 (9)	C9—C10	1.369 (6)
Ni1—P1	2.2014 (8)	C9—H9	0.9300
Ni1—S2	2.2371 (9)	C10—C11	1.353 (6)
P1—C1	1.822 (3)	C10—H10	0.9300
P1—C7	1.826 (3)	C11—C12	1.389 (5)
P1—C13	1.833 (3)	C11—H11	0.9300
S1—C15	1.722 (3)	C12—H12	0.9300
S2—C15	1.713 (3)	C13—C14	1.501 (5)
N1—C15	1.295 (4)	C13—H13A	0.9700
N1—C16	1.468 (5)	C13—H13B	0.9700
N1—C19	1.477 (4)	C14—H14A	0.9600
C1—C2	1.386 (4)	C14—H14B	0.9600
C1—C6	1.386 (4)	C14—H14C	0.9600
C2—C3	1.385 (5)	C16—C17	1.453 (6)
C2—H2	0.9300	C16—H16A	0.9700
C3—C4	1.375 (6)	C16—H16B	0.9700
C3—H3	0.9300	C17—C18	1.420 (7)
C4—C5	1.362 (6)	C17—H17A	0.9700
C4—H4	0.9300	C17—H17B	0.9700
C5—C6	1.377 (5)	C18—C19	1.488 (5)
C5—H5	0.9300	C18—H18A	0.9700
C6—H6	0.9300	C18—H18B	0.9700
C7—C12	1.371 (5)	C19—H19A	0.9700
C7—C8	1.382 (5)	C19—H19B	0.9700
C8—C9	1.375 (5)		
S1—Ni1—C11	170.25 (4)	C9—C10—H10	120.3
S1—Ni1—P1	94.10 (3)	C10—C11—C12	121.1 (4)
C11—Ni1—P1	94.62 (3)	C10—C11—H11	119.5
S1—Ni1—S2	78.70 (3)	C12—C11—H11	119.5
C11—Ni1—S2	92.99 (4)	C7—C12—C11	120.1 (4)
P1—Ni1—S2	171.11 (4)	C7—C12—H12	120.0
C1—P1—C7	102.11 (14)	C11—C12—H12	120.0
C1—P1—C13	104.01 (16)	C14—C13—P1	116.0 (3)
C7—P1—C13	103.83 (16)	C14—C13—H13A	108.3
C1—P1—Ni1	113.44 (9)	P1—C13—H13A	108.3

C7—P1—Ni1	116.52 (10)	C14—C13—H13B	108.3
C13—P1—Ni1	115.28 (14)	P1—C13—H13B	108.3
C15—S1—Ni1	86.65 (11)	H13A—C13—H13B	107.4
C15—S2—Ni1	85.09 (11)	C13—C14—H14A	109.5
C15—N1—C16	124.2 (3)	C13—C14—H14B	109.5
C15—N1—C19	124.4 (3)	H14A—C14—H14B	109.5
C16—N1—C19	111.4 (3)	C13—C14—H14C	109.5
C2—C1—C6	118.3 (3)	H14A—C14—H14C	109.5
C2—C1—P1	119.8 (2)	H14B—C14—H14C	109.5
C6—C1—P1	121.9 (2)	N1—C15—S2	125.9 (2)
C3—C2—C1	120.6 (3)	N1—C15—S1	124.7 (2)
C3—C2—H2	119.7	S2—C15—S1	109.28 (18)
C1—C2—H2	119.7	C17—C16—N1	104.2 (3)
C4—C3—C2	119.9 (4)	C17—C16—H16A	110.9
C4—C3—H3	120.1	N1—C16—H16A	110.9
C2—C3—H3	120.1	C17—C16—H16B	110.9
C5—C4—C3	120.1 (4)	N1—C16—H16B	110.9
C5—C4—H4	119.9	H16A—C16—H16B	108.9
C3—C4—H4	119.9	C18—C17—C16	111.2 (4)
C4—C5—C6	120.3 (4)	C18—C17—H17A	109.4
C4—C5—H5	119.8	C16—C17—H17A	109.4
C6—C5—H5	119.8	C18—C17—H17B	109.4
C5—C6—C1	120.8 (4)	C16—C17—H17B	109.4
C5—C6—H6	119.6	H17A—C17—H17B	108.0
C1—C6—H6	119.6	C17—C18—C19	108.8 (4)
C12—C7—C8	118.2 (3)	C17—C18—H18A	109.9
C12—C7—P1	121.3 (3)	C19—C18—H18A	109.9
C8—C7—P1	120.4 (3)	C17—C18—H18B	109.9
C9—C8—C7	121.1 (4)	C19—C18—H18B	109.9
C9—C8—H8	119.4	H18A—C18—H18B	108.3
C7—C8—H8	119.4	N1—C19—C18	103.6 (3)
C10—C9—C8	120.1 (4)	N1—C19—H19A	111.0
C10—C9—H9	120.0	C18—C19—H19A	111.0
C8—C9—H9	120.0	N1—C19—H19B	111.0
C11—C10—C9	119.4 (4)	C18—C19—H19B	111.0
C11—C10—H10	120.3	H19A—C19—H19B	109.0