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Chlorido(4-morpholinecarbodithioato-κ^2S,S')(triphenylphosphine)nickel(II)

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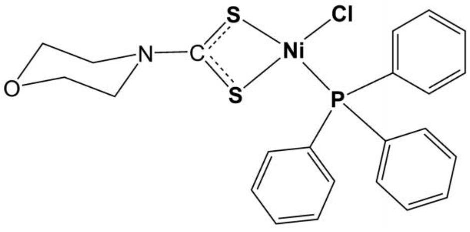
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.003 Å; R factor = 0.027; wR factor = 0.079; data-to-parameter ratio = 16.4.

The title complex, [Ni(C$_5$H$_8$NOS$_2$)Cl(C$_{18}$H$_{15}$P)], exhibits a four-coordinate Ni atom in a slightly distorted square-planar geometry.

Related literature

For related literature, see: Allen (2002); Garton *et al.* (1963); Pastorek *et al.* (1996, 1999); Pavlicek *et al.* (2003); Shaheen *et al.* (2006).



Experimental

Crystal data

[Ni(C$_5$H$_8$NOS$_2$)Cl(C$_{18}$H$_{15}$P)]
M_r = 518.67
Triclinic, $P\bar{1}$
a = 9.4814 (8) Å
b = 10.6009 (9) Å
c = 13.243 (1) Å
α = 111.908 (8)°
β = 91.044 (7)°
γ = 110.924 (8)°
V = 1135.7 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.24 mm^{-1}
T = 120 (2) K
0.24 × 0.16 × 0.06 mm

Data collection

Oxford Diffraction KM-4-CCD diffractometer
Absorption correction: analytical [*CrysAlis RED* (Oxford Diffraction, 2006); analytical numeric absorption correction using a multifaceted crystal model (Clark & Reid, 1995)]
$T_{\rm min}$ = 0.621, $T_{\rm max}$ = 0.843
8344 measured reflections
4448 independent reflections
4283 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.011

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.079
S = 1.13
4448 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max}$ = 0.56 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.37 e Å^{-3}

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; 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) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IM2015).

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supplementary materials

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Chlorido(4-morpholinecarbodithioato-$\kappa^2 S,S'$)(triphenylphosphine)nickel(II)

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Comment

Dithiocarbamates have been studied extensively over recent decades in response to their growing applications in many areas such as industry, biology and analytical chemistry. The *N,N*-disubstituted dithiocarbamate residue (dtc) is the classical bidentate ligand and one of the most frequently used sulfur donors (Cambridge Structural Database, 2007 with updates; Allen, 2002). Recently we began to devote our interest to Ni complexes where this ligand is simultaneously accompanied by a halogene and phosphine.

Here we describe a new product - (4-morpholinecarbodithioato-*S*,*S*')-chloro-(triphenylphosphine)-nickel(II)(**I**) (Scheme I) obtained by essentially quantitative metathesis of *trans*-dichloro-bis(triphenylphosphine)-nickel(II) (Garton *et al.*, 1963) and bis(4-morpholinecarbodithioato-S,*S*') nickel(II) prepared *in situ*.

For our purposes we have chosen a dithiocarbamate ligand derived from a cyclic amine. Interestingly, only a few complexes of this kind have been structurally characterized. For Ni four such compounds may be quoted, among them two containing a chloro (Pastorek *et al.*, 1999, Pavlicek *et al.*, 2003) and two with a bromo ligand (Pastorek *et al.*, 1996, Pavlicek *et al.*, 2003). In addition, one Pd containing complex has recently been described (Shaheen *et al.*, 2006).

The molecular structure of (**I**) with atom numbering scheme is shown in Fig.1. The single-crystal X-ray analysis proved, as expected, a distorted square-planar arrangement of the NiS_2ClP complex core. The dtc ligand acts as a bidentate chelating ligand, coordinating to Ni *via* both S atoms. Atom S1 is located *trans* to the triphenylphosphine ligand and atom S2 is *trans* to the Cl ligand. The slight deformation of the coordination geometry is probably caused by the presence of both chelating agent and sterically hindered phosphine.

It is noteworthy that (**I**) which was recrystallized from chloroform as were all four aforementioned Ni complexes, does not retain the solvent within its crystal structure. It therefore resembles the Pd-containing complex, which was crystallized from dichloromethane and obviously does not contain chloroform.

A closer look at (**I**) reveals some short contacts $C_{morph}H\cdots Cl$, within a pair of molecules (Fig. 2), which may suggest that some additional weak interractions are present. This corresponds to the slightly longer Ni—Cl bond length and smaller P—Ni—Cl angle comparing to the previously mentioned species.

Experimental

Nickel chloride, $NiCl_2 \times 6H_2O$ (0.608 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 potassium salt of 4-morpholinecarbodithioic acid $OC_4H_8NCS_2K$ (1.03 g, 0.005 mol) dissolved in methanol/water. The mixture was stirred vigorously in an inert gas (Ar) atmosphere for 30 minutes, then filtered and left for crystallization at 5° C. After *ca*. two weeks green crystalline product, namely $Ni(S_2CNC_4H_8O)_2$ was collected. It was again dissolved (0.206 g, 0.00058 mol) in 10 ml of chloroform and mixed with solution of equimolar amount of $NiCl_2(PPh_3)_2$ (0.379 g). The mixture which turned to deep violet, was stirred for 10 minutes and then filtered. To the solution 10 ml of Et_2O was added. After15 minutes crimson-violet crystals were collected and washed with several portions of ether.

Refinement

All H atoms were placed in calculated positions (0.95 Å for CH aryl and 0.99 Å for CH_2 alkyl) and refined as riding with $U_{iso}(H) = 1.2U_{eq}$ (aryl carrier) or $1.3U_{eq}$ (methylene carrier).

Figures

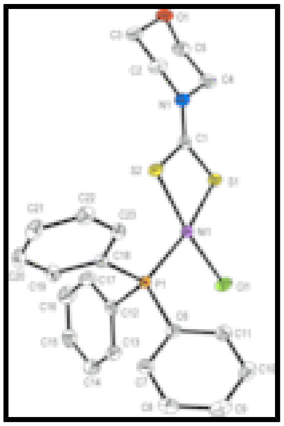

Fig. 1. Molecular structure and atom-numbering scheme for **I** with displacement ellipsoids drawn at the 50% probability level.

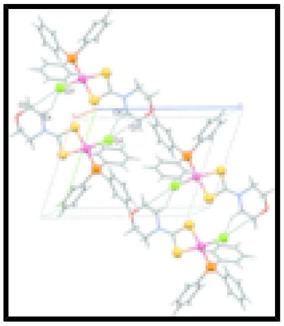

Fig. 2. Schematic drawing of the crystal packing of **I** showing short contacts within a pair of molecules. (C4···Cl1' 3.581 Å, C5···Cl1' 3.432 Å)

Chlorido(4-morpholinecarbodithioato- κ^2*S*,*S*')(triphenylphosphine)nickel(II)

Crystal data

$[Ni(C_5H_8NOS_2)Cl(C_{18}H_{15}P)]$	$Z = 2$
$M_r = 518.67$	$F_{000} = 536$
Triclinic, $P\overline{1}$	$D_x = 1.517$ Mg m^{-3}
Hall symbol: -P 1	Mo *K*α radiation λ = 0.71073 Å
a = 9.4814 (8) Å	Cell parameters from 10672 reflections
b = 10.6009 (9) Å	θ = 2.2–32.4°
c = 13.243 (1) Å	μ = 1.24 mm^{-1}
α = 111.908 (8)°	*T* = 120 (2) K

β = 91.044 (7)°
γ = 110.924 (8)°
V = 1135.7 (2) Å^3

Prism, crimson-violet
0.24 × 0.16 × 0.06 mm

Data collection

4-axis κ geometry diffractometer
Monochromator: graphite
Detector resolution: 8.1883 pixels mm^{-1}
T = 120(2) K
ω scans, 0.75° width
Absorption correction: analytical [CrysAlis RED (Oxford Diffraction, 2006); analytical numeric absorption correction using a multifaceted crystal model (Clark & Reid, 1995)]
T_{min} = 0.621, T_{max} = 0.843
8344 measured reflections

4448 independent reflections
4283 reflections with $I > 2\sigma(I)$
R_{int} = 0.011
θ_{max} = 26°
θ_{min} = 2.2°
$h = -11 \rightarrow 9$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 16$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.079
S = 1.13
4448 reflections
271 parameters
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
$w = 1/[\sigma^2(F_o^2) + (0.0476P)^2 + 0.6214P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\mathrm{max}} < 0.001$
$\Delta\rho_{\mathrm{max}}$ = 0.56 e Å^{-3}
$\Delta\rho_{\mathrm{min}}$ = −0.37 e Å^{-3}
Extinction correction: none

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}

Ni1	0.71797 (2)	0.33190 (2)	0.119811 (16)	0.01561 (8)
Cl1	0.68831 (5)	0.24822 (5)	0.24958 (3)	0.02355 (11)
S1	0.68647 (5)	0.11482 (5)	−0.01212 (3)	0.01960 (11)
S2	0.75229 (5)	0.38803 (5)	−0.02326 (3)	0.01922 (11)
P1	0.70778 (5)	0.53984 (5)	0.23183 (3)	0.01527 (10)
O1	0.64896 (15)	0.00309 (15)	−0.43865 (10)	0.0268 (3)
N1	0.71309 (16)	0.14260 (16)	−0.20607 (12)	0.0206 (3)
C1	0.71688 (18)	0.20381 (19)	−0.09929 (14)	0.0178 (3)
C2	0.7558 (2)	0.2294 (2)	−0.27353 (14)	0.0236 (4)
H2A	0.8629	0.247	−0.285	0.031*
H2B	0.7495	0.3265	−0.2343	0.031*
C3	0.6494 (2)	0.1474 (2)	−0.38444 (14)	0.0246 (4)
H3A	0.5442	0.1398	−0.3734	0.032*
H3B	0.6836	0.2031	−0.4312	0.032*
C4	0.6860 (2)	−0.0152 (2)	−0.26313 (15)	0.0239 (4)
H4A	0.6346	−0.0691	−0.2183	0.031*
H4B	0.7852	−0.0257	−0.2723	0.031*
C5	0.5861 (2)	−0.0805 (2)	−0.37556 (15)	0.0275 (4)
H5A	0.5764	−0.1835	−0.4164	0.036*
H5B	0.4823	−0.0825	−0.3655	0.036*
C6	0.83379 (19)	0.64355 (18)	0.36638 (13)	0.0174 (3)
C7	0.8329 (2)	0.77928 (19)	0.43852 (14)	0.0215 (3)
H7	0.7631	0.8155	0.4188	0.026*
C8	0.9336 (2)	0.8608 (2)	0.53860 (15)	0.0248 (4)
H8	0.9319	0.9523	0.5874	0.03*
C9	1.0368 (2)	0.8096 (2)	0.56801 (15)	0.0254 (4)
H9	1.1056	0.8658	0.6366	0.03*
C10	1.0392 (2)	0.6759 (2)	0.49680 (15)	0.0231 (4)
H10	1.1098	0.6407	0.5167	0.028*
C11	0.93838 (19)	0.59321 (19)	0.39625 (14)	0.0195 (3)
H11	0.9408	0.5019	0.3477	0.023*
C12	0.51067 (19)	0.49114 (18)	0.25703 (14)	0.0185 (3)
C13	0.4727 (2)	0.5150 (2)	0.36186 (15)	0.0244 (4)
H13	0.5516	0.5664	0.425	0.029*
C14	0.3195 (2)	0.4639 (2)	0.37452 (17)	0.0300 (4)
H14	0.2945	0.4804	0.4462	0.036*
C15	0.2038 (2)	0.3891 (2)	0.28266 (17)	0.0283 (4)
H15	0.0995	0.3535	0.2913	0.034*
C16	0.2406 (2)	0.3662 (2)	0.17825 (17)	0.0297 (4)
H16	0.1613	0.3164	0.1154	0.036*
C17	0.3933 (2)	0.4161 (2)	0.16519 (15)	0.0252 (4)
H17	0.4178	0.399	0.0933	0.03*
C18	0.74246 (18)	0.68505 (18)	0.18132 (13)	0.0164 (3)
C19	0.64409 (19)	0.75773 (19)	0.18590 (14)	0.0203 (3)
H19	0.5491	0.7262	0.2102	0.024*
C20	0.6844 (2)	0.8761 (2)	0.15500 (16)	0.0243 (4)
H20	0.6165	0.9245	0.1577	0.029*
C21	0.8233 (2)	0.9237 (2)	0.12022 (15)	0.0242 (4)
H21	0.8521	1.0067	0.1017	0.029*

C22	0.9203 (2)	0.8495 (2)	0.11252 (15)	0.0225 (4)
H22	1.0142	0.8803	0.0868	0.027*
C23	0.87987 (19)	0.73035 (19)	0.14237 (14)	0.0188 (3)
H23	0.9459	0.6794	0.1363	0.023*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.01970 (13)	0.01613 (13)	0.01347 (12)	0.00895 (9)	0.00388 (9)	0.00673 (9)
Cl1	0.0342 (2)	0.0194 (2)	0.0179 (2)	0.00850 (17)	0.00356 (17)	0.01034 (16)
S1	0.0269 (2)	0.0181 (2)	0.0159 (2)	0.01110 (17)	0.00499 (16)	0.00700 (16)
S2	0.0254 (2)	0.0184 (2)	0.0147 (2)	0.00875 (17)	0.00347 (16)	0.00747 (16)
P1	0.0180 (2)	0.0169 (2)	0.0138 (2)	0.00887 (16)	0.00428 (15)	0.00719 (16)
O1	0.0284 (7)	0.0323 (7)	0.0155 (6)	0.0111 (6)	0.0052 (5)	0.0059 (5)
N1	0.0200 (7)	0.0219 (7)	0.0187 (7)	0.0068 (6)	0.0041 (6)	0.0084 (6)
C1	0.0146 (7)	0.0203 (8)	0.0190 (8)	0.0070 (6)	0.0019 (6)	0.0083 (7)
C2	0.0231 (9)	0.0272 (9)	0.0168 (8)	0.0047 (7)	0.0026 (7)	0.0100 (7)
C3	0.0241 (9)	0.0315 (10)	0.0161 (8)	0.0101 (7)	0.0033 (7)	0.0082 (7)
C4	0.0273 (9)	0.0235 (9)	0.0177 (8)	0.0108 (7)	0.0045 (7)	0.0042 (7)
C5	0.0291 (9)	0.0266 (9)	0.0191 (9)	0.0084 (8)	0.0034 (7)	0.0036 (7)
C6	0.0200 (8)	0.0192 (8)	0.0145 (7)	0.0072 (6)	0.0048 (6)	0.0088 (6)
C7	0.0257 (8)	0.0220 (9)	0.0195 (8)	0.0115 (7)	0.0067 (7)	0.0091 (7)
C8	0.0305 (9)	0.0208 (9)	0.0195 (8)	0.0081 (7)	0.0084 (7)	0.0062 (7)
C9	0.0242 (9)	0.0268 (9)	0.0171 (8)	0.0011 (7)	0.0009 (7)	0.0092 (7)
C10	0.0211 (8)	0.0277 (9)	0.0233 (9)	0.0076 (7)	0.0025 (7)	0.0154 (7)
C11	0.0211 (8)	0.0201 (8)	0.0192 (8)	0.0077 (7)	0.0053 (6)	0.0104 (7)
C12	0.0195 (8)	0.0183 (8)	0.0212 (8)	0.0089 (6)	0.0064 (6)	0.0100 (7)
C13	0.0245 (9)	0.0329 (10)	0.0206 (9)	0.0139 (8)	0.0055 (7)	0.0132 (7)
C14	0.0297 (10)	0.0449 (12)	0.0282 (10)	0.0203 (9)	0.0150 (8)	0.0224 (9)
C15	0.0216 (9)	0.0340 (10)	0.0397 (11)	0.0135 (8)	0.0115 (8)	0.0230 (9)
C16	0.0218 (9)	0.0333 (10)	0.0302 (10)	0.0070 (8)	0.0015 (7)	0.0127 (8)
C17	0.0244 (9)	0.0295 (9)	0.0196 (8)	0.0095 (7)	0.0047 (7)	0.0087 (7)
C18	0.0187 (8)	0.0168 (8)	0.0139 (7)	0.0080 (6)	0.0016 (6)	0.0055 (6)
C19	0.0192 (8)	0.0212 (8)	0.0221 (8)	0.0094 (7)	0.0039 (7)	0.0089 (7)
C20	0.0239 (9)	0.0224 (9)	0.0300 (9)	0.0127 (7)	0.0004 (7)	0.0109 (7)
C21	0.0249 (9)	0.0212 (8)	0.0270 (9)	0.0060 (7)	−0.0012 (7)	0.0134 (7)
C22	0.0185 (8)	0.0255 (9)	0.0224 (9)	0.0055 (7)	0.0015 (7)	0.0116 (7)
C23	0.0178 (8)	0.0217 (8)	0.0183 (8)	0.0091 (6)	0.0022 (6)	0.0085 (7)

Geometric parameters (Å, °)

Ni1—S2	2.1852 (5)	C8—H8	0.95
Ni1—P1	2.1877 (5)	C9—C10	1.387 (3)
Ni1—Cl1	2.1900 (5)	C9—H9	0.95
Ni1—S1	2.2197 (5)	C10—C11	1.393 (2)
S1—C1	1.7136 (17)	C10—H10	0.95
S2—C1	1.7298 (18)	C11—H11	0.95
P1—C12	1.8256 (17)	C12—C13	1.393 (2)
P1—C6	1.8258 (17)	C12—C17	1.395 (3)

P1—C18	1.8275 (17)	C13—C14	1.395 (3)
O1—C5	1.425 (2)	C13—H13	0.95
O1—C3	1.426 (2)	C14—C15	1.387 (3)
N1—C1	1.311 (2)	C14—H14	0.95
N1—C2	1.473 (2)	C15—C16	1.386 (3)
N1—C4	1.476 (2)	C15—H15	0.95
C2—C3	1.516 (2)	C16—C17	1.392 (3)
C2—H2A	0.99	C16—H16	0.95
C2—H2B	0.99	C17—H17	0.95
C3—H3A	0.99	C18—C19	1.396 (2)
C3—H3B	0.99	C18—C23	1.399 (2)
C4—C5	1.518 (3)	C19—C20	1.391 (2)
C4—H4A	0.99	C19—H19	0.95
C4—H4B	0.99	C20—C21	1.386 (3)
C5—H5A	0.99	C20—H20	0.95
C5—H5B	0.99	C21—C22	1.391 (3)
C6—C11	1.395 (2)	C21—H21	0.95
C6—C7	1.402 (2)	C22—C23	1.389 (2)
C7—C8	1.387 (3)	C22—H22	0.95
C7—H7	0.95	C23—H23	0.95
C8—C9	1.389 (3)		

S2—Ni1—P1	96.597 (18)	C6—C7—H7	119.9
S2—Ni1—Cl1	172.162 (18)	C7—C8—C9	120.50 (17)
P1—Ni1—Cl1	91.198 (18)	C7—C8—H8	119.8
S2—Ni1—S1	78.878 (18)	C9—C8—H8	119.8
P1—Ni1—S1	168.831 (19)	C10—C9—C8	119.73 (17)
Cl1—Ni1—S1	93.595 (18)	C10—C9—H9	120.1
C1—S1—Ni1	85.84 (6)	C8—C9—H9	120.1
C1—S2—Ni1	86.54 (6)	C9—C10—C11	120.21 (16)
C12—P1—C6	107.31 (8)	C9—C10—H10	119.9
C12—P1—C18	105.46 (7)	C11—C10—H10	119.9
C6—P1—C18	101.02 (7)	C10—C11—C6	120.40 (16)
C12—P1—Ni1	105.29 (6)	C10—C11—H11	119.8
C6—P1—Ni1	119.15 (6)	C6—C11—H11	119.8
C18—P1—Ni1	117.59 (5)	C13—C12—C17	119.06 (16)
C5—O1—C3	109.06 (13)	C13—C12—P1	123.20 (14)
C1—N1—C2	122.46 (15)	C17—C12—P1	117.55 (13)
C1—N1—C4	121.45 (15)	C12—C13—C14	120.36 (18)
C2—N1—C4	115.58 (14)	C12—C13—H13	119.8
N1—C1—S1	125.79 (14)	C14—C13—H13	119.8
N1—C1—S2	125.49 (13)	C15—C14—C13	120.13 (17)
S1—C1—S2	108.72 (10)	C15—C14—H14	119.9
N1—C2—C3	110.18 (14)	C13—C14—H14	119.9
N1—C2—H2A	109.6	C16—C15—C14	119.83 (17)
C3—C2—H2A	109.6	C16—C15—H15	120.1
N1—C2—H2B	109.6	C14—C15—H15	120.1
C3—C2—H2B	109.6	C15—C16—C17	120.21 (18)
H2A—C2—H2B	108.1	C15—C16—H16	119.9
O1—C3—C2	110.34 (15)	C17—C16—H16	119.9

O1—C3—H3A	109.6
C2—C3—H3A	109.6
O1—C3—H3B	109.6
C2—C3—H3B	109.6
H3A—C3—H3B	108.1
N1—C4—C5	109.61 (15)
N1—C4—H4A	109.7
C5—C4—H4A	109.7
N1—C4—H4B	109.7
C5—C4—H4B	109.7
H4A—C4—H4B	108.2
O1—C5—C4	111.48 (15)
O1—C5—H5A	109.3
C4—C5—H5A	109.3
O1—C5—H5B	109.3
C4—C5—H5B	109.3
H5A—C5—H5B	108
C11—C6—C7	119.04 (16)
C11—C6—P1	120.51 (13)
C7—C6—P1	120.35 (13)
C8—C7—C6	120.13 (16)
C8—C7—H7	119.9
C16—C17—C12	120.40 (17)
C16—C17—H17	119.8
C12—C17—H17	119.8
C19—C18—C23	119.05 (15)
C19—C18—P1	123.48 (13)
C23—C18—P1	117.36 (12)
C20—C19—C18	120.33 (16)
C20—C19—H19	119.8
C18—C19—H19	119.8
C21—C20—C19	120.26 (16)
C21—C20—H20	119.9
C19—C20—H20	119.9
C20—C21—C22	119.84 (16)
C20—C21—H21	120.1
C22—C21—H21	120.1
C23—C22—C21	120.07 (16)
C23—C22—H22	120
C21—C22—H22	120
C22—C23—C18	120.39 (15)
C22—C23—H23	119.8
C18—C23—H23	119.8

Fig. 1

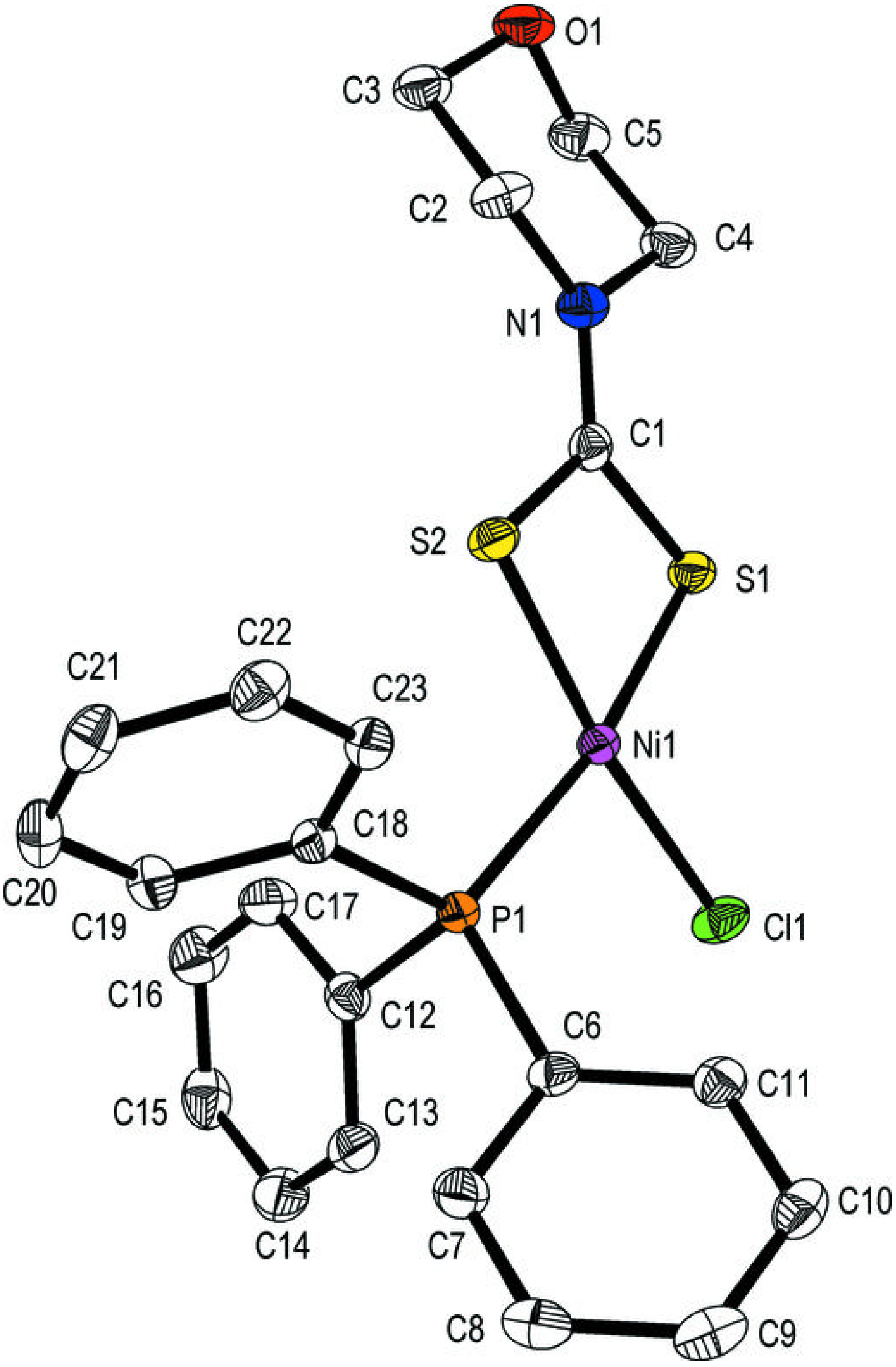
O1
C3
C5
C2
C4
N1
C1
S2
S1
C22
C21
C23
Ni1
C18
C20
C17
C19
P1
Cl1
C16
C12
C6
C11
C15
C13
C10
C7
C14
C8
C9

Fig. 2