

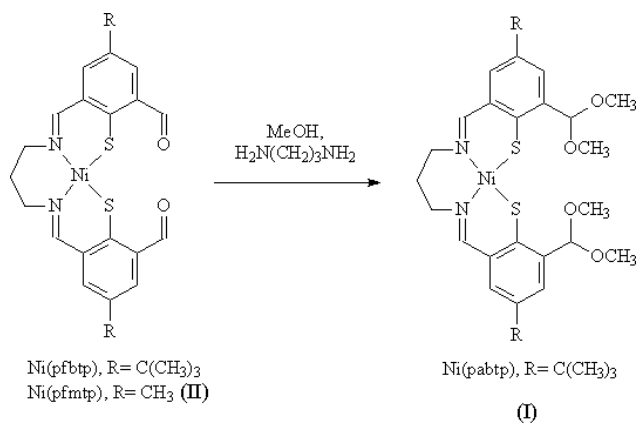
Jens K. Bjernemose,<sup>a</sup> Christine J. McKenzie,<sup>a\*</sup> Paul R. Raithby<sup>b</sup> and Simon J. Teat<sup>c</sup><sup>a</sup>Department of Chemistry, University of Southern Denmark, Campusvej 55, DK-5230 Odense M, Denmark, <sup>b</sup>Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, England, and <sup>c</sup>CLRC Daresbury Laboratory, Daresbury, Warrington WA4 4AD, England

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## Key indicators

Single-crystal synchrotron study  
T = 150 K  
Mean  $\sigma(C-C)$  = 0.004 Å  
R factor = 0.084  
wR factor = 0.228  
Data-to-parameter ratio = 53.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**{4,4'-Di-*tert*-butyl-6,6'-bis(dimethoxymethyl)-2,2'-[propane-1,3-diylbis(nitrilomethylidene)]-bis(thiophenolato)- $\kappa^4$ S,N,N',S'}nickel(II)**The title compound, [Ni(C<sub>31</sub>H<sub>44</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub>)], is an N<sub>2</sub>S<sub>2</sub> four-coordinated nickel(II) complex. The coordination geometry of the metal, on a twofold rotation axis, is more distorted from square planar than in related compounds.Received 11 October 2004  
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## Comment

The title compound, Ni(pabtp), (I), was isolated from a mixture of the dialdehyde [*N,N'*-propane-1,3-diyl(6-formyl-4-*tert*-butyl-2-methyliminatothiophenolato)]nickel(II) (Christensen & McKenzie, 2004), Ni(pfbtp) and 1,3-diaminopropane in methanol (see scheme). This reaction was an unsuccessful attempt to prepare a ring-closed Schiff base derivative of Ni(pfbtp) under conditions analogous to those in which we prepared 2 + 2 and 4 + 4 thiophenolate macrocyclic complexes using Ni(pfmp), (II), which is homologous to Ni(pfbtp) [Cambridge Structural Database, Version 5.25 of November 2003 with three updates (Allen, 2002) reocode NULPOZ; Christensen *et al.*, 1997].Comparing (I) and (II), it is immediately evident that no change in the length of the coordinating bonds has occurred, but although the coordination geometry at the Ni atom in (I) may be described as square planar, it is far more distorted towards tetrahedral than in (II). This can be seen from the change in bond angles around the Ni atom, which lies on a twofold rotation axis, but is more strikingly described by looking at the volume of the (irregular) tetrahedron spanned by the four donor atoms (N<sub>2</sub>S<sub>2</sub>). This is 1.544 Å<sup>3</sup> for (I) but only 0.159 Å<sup>3</sup> for (II). A space-filling model shows no direct interaction between the two (MeO)<sub>2</sub>CH— groups on either side of the Ni atom, thus this distortion from square planar is apparently not due to the bulkier dimethylacetal groups replacing the formyl groups. The distortion is then more likely to be due to packing effects. Inspection of the packing diagrams for (I) and (II) reveals a number of similarities. The

molecules in (I) essentially stack along *c*, alternating their direction in either layer, but, whereas molecules in (II) have the Ni atoms directly above one another, they are more displaced in (I). These stacks then pack in a head-to-tail fashion along *b*, with the central methylene group nestled between the two S atoms of the next molecule [ $C-H \cdots S = 3.64 \text{ \AA}$  compared to  $3.20 \text{ \AA}$  in (II)]. These *ab* layers then have *tert*-butyl groups on both sides along *c* in (I) [methyl groups in the case of (II)]. This is probably the origin of the distortion around Ni, for while (II) shows only very modest interaction between the methyl and formyl groups, (I) has a much closer approach of the *tert*-butyl groups to the dimethoxymethyl group.

## Experimental

Crystals of (I) were isolated from a 1:1 mixture of Ni(pfbtp) (Christensen & McKenzie, 2004) and 1,3-diaminopropane in methanol after several days standing in a closed vessel.

### Crystal data

[Ni(C <sub>31</sub> H <sub>44</sub> N <sub>2</sub> O <sub>4</sub> S <sub>2</sub> )]	Synchrotron radiation
<i>M<sub>r</sub></i> = 631.51	$\lambda = 0.6881 \text{ \AA}$
Monoclinic, <i>C2/c</i>	Cell parameters from 6249 reflections
<i>a</i> = 28.352 (4) $\text{\AA}$	$\theta = 2.8\text{--}29.2^\circ$
<i>b</i> = 9.1532 (11) $\text{\AA}$	$\mu = 0.80 \text{ mm}^{-1}$
<i>c</i> = 12.1556 (15) $\text{\AA}$	<i>T</i> = 150 (2) K
$\beta = 102.178 (2)^\circ$	Needle, orange-red
<i>V</i> = 3083.5 (7) $\text{\AA}^3$	0.22 × 0.02 × 0.01 mm
<i>Z</i> = 4	
<i>D<sub>x</sub></i> = 1.36 Mg m <sup>-3</sup>	

### Data collection

Bruker SMART 1K CCD diffractometer	9981 independent reflections
$\omega$ scans	8220 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2000)	$\theta_{\text{max}} = 27.5^\circ$
$T_{\text{min}} = 0.843$ , $T_{\text{max}} = 0.992$	$h = -37 \rightarrow 38$
9981 measured reflections	$k = -12 \rightarrow 12$
	$l = -16 \rightarrow 16$

### Refinement

Refinement on $F^2$	$w = 1/[\sigma^2(F_o^2) + (0.169P)^2 + 0.2945P]$
$R[F^2 > 2\sigma(F^2)] = 0.084$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.228$	$(\Delta/\sigma)_{\text{max}} < 0.001$
<i>S</i> = 1.04	$\Delta\rho_{\text{max}} = 1.77 \text{ e \AA}^{-3}$
9981 reflections	$\Delta\rho_{\text{min}} = -1.23 \text{ e \AA}^{-3}$
188 parameters	
H-atom parameters constrained	

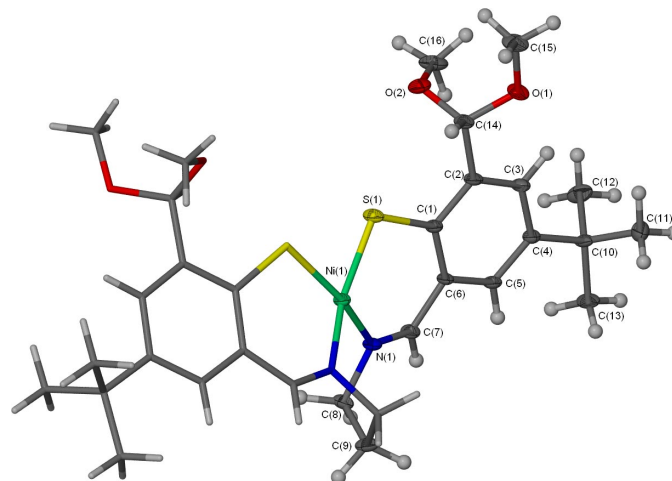
**Table 1**

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

Ni1—N1	1.907 (2)	Ni1—S1	2.1742 (8)
N1—Ni1—N1 <sup>1</sup>	90.49 (14)	N1—Ni1—S1	95.30 (7)
N1—Ni1—S1 <sup>1</sup>	163.52 (7)	S1 <sup>1</sup> —Ni1—S1	83.41 (4)

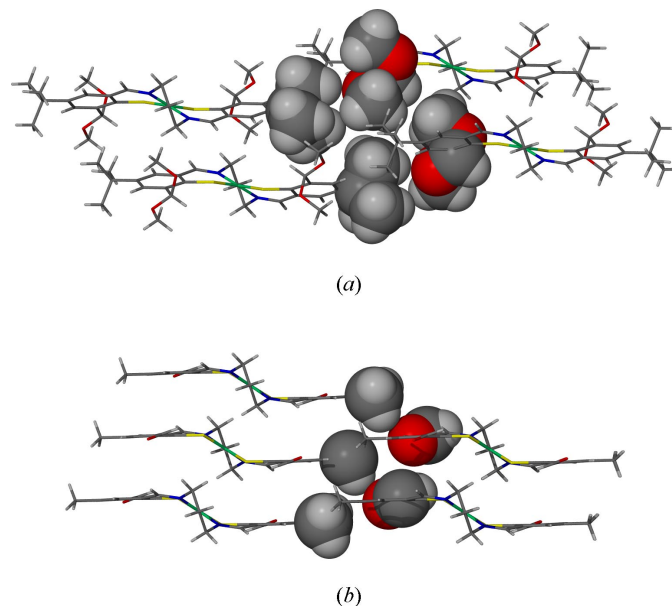
Symmetry code: (i)  $-x, y, \frac{1}{2} - z$ .

The crystals turned out to be twinned. *ROTAX* (Parsons & Gould, 2001) identifies the twinning as  $180^\circ$  rotation about the *a* axis. The twin scale is  $[101, 0\bar{1}0, 00\bar{1}]$ . The batch scale factor refines to 0.2786 (18). The non-merohedral twinning prevents merging of equivalent reflections before refinement. The maximum and minimum electron-density peaks are located 0.88 and 0.76  $\text{\AA}$ , respectively, from atom Ni1.



**Figure 1**

View of (I), with 50% probability displacement ellipsoids shown only for atoms of the asymmetric unit. Unlabelled atoms are related to labelled atoms by  $-x, y, 1/2 - z$ .



**Figure 2**

The packing of (a) Ni(pabtp), (I), (b) Ni(pfmp), (II). View down *b* with *tert*-butyl (a) or methyl (b) groups shown as space-filling on the left and dimethoxymethyl (a) or formyl (b) groups on the right.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINTE* (Bruker, 2000); data reduction: *SAINTE*; program(s) used to solve structure: *DIRDIF99* (Beurskens *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-Seed* (Barbour, 2001); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

We are grateful to the CCLRC Daresbury Laboratory for the award of beamtime to carry out the diffraction experiment.

## References

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## supporting information

*Acta Cryst.* (2004). E60, m1841–m1843 [https://doi.org/10.1107/S1600536804028879]

**{4,4'-Di-*tert*-butyl-6,6'-bis(dimethoxymethyl)-2,2'-[propane-1,3-diylbis(nitrilomethylidyne)]bis(thiophenolato)- $\kappa^4$ S,N,N',S'}nickel(II)**

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*Crystal data*

[Ni(C<sub>31</sub>H<sub>44</sub>N<sub>2</sub>O<sub>4</sub>S<sub>2</sub>)]

$M_r = 631.51$

Monoclinic, *C2/c*

Hall symbol: -C 2yc

$a = 28.352$  (4) Å

$b = 9.1532$  (11) Å

$c = 12.1556$  (15) Å

$\beta = 102.178$  (2)°

$V = 3083.5$  (7) Å<sup>3</sup>

$Z = 4$

$F(000) = 1344$

$D_x = 1.36$  Mg m<sup>-3</sup>

Synchrotron radiation,  $\lambda = 0.6881$  Å

Cell parameters from 6249 reflections

$\theta = 2.8$ – $29.2$ °

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$T = 150$  K

Needle, orange-red

$0.22 \times 0.02 \times 0.01$  mm

*Data collection*

Bruker SMART 1K CCD

diffractometer

Radiation source: Synchrotron, SRS station 9.8

Graphite monochromator

$0.20$ °  $\omega$  rotation, 3 s a frame scans

Absorption correction: multi-scan

(SADABS; Bruker, 2000)

$T_{\min} = 0.843$ ,  $T_{\max} = 0.992$

9981 measured reflections

9981 independent reflections

8220 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0$

$\theta_{\max} = 27.5$ °,  $\theta_{\min} = 2.3$ °

$h = -37$ → $38$

$k = -12$ → $12$

$l = -16$ → $16$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.084$

$wR(F^2) = 0.228$

$S = 1.04$

9981 reflections

188 parameters

0 restraints

Primary atom site location: heavy-atom method

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.169P)^2 + 0.2945P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 1.77$  e Å<sup>-3</sup>

$\Delta\rho_{\min} = -1.23$  e Å<sup>-3</sup>

*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.

The crystals turn out to be twinned. ROTAX (Parsons & Gould, 2001) identifies the twinning as  $180^\circ$  rotation about  $\{1\ 0\ 0\}$  ( $a^-$ ). The corresponding twin law is  $[1\ 0\ 1]\ [0\ -1\ 0]\ [0\ 0\ -1]$  The batch scale factor refines to 0.27859

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$	Occ. (<1)
C1	0.07866 (9)	0.1434 (3)	0.1114 (2)	0.0182 (5)	
C2	0.11604 (9)	0.2375 (3)	0.0921 (3)	0.0201 (5)	
C3	0.15119 (10)	0.1872 (3)	0.0375 (2)	0.0208 (5)	
H3	0.1764	0.2519	0.0289	0.025*	
C4	0.15123 (10)	0.0449 (3)	-0.0057 (3)	0.0195 (5)	
C5	0.11417 (10)	-0.0464 (3)	0.0113 (3)	0.0200 (5)	
H5	0.1125	-0.1428	-0.0182	0.024*	
C6	0.07905 (10)	-0.0017 (3)	0.0706 (3)	0.0190 (6)	
C7	0.04429 (9)	-0.1128 (3)	0.0840 (2)	0.0208 (6)	
H7	0.0434	-0.1973	0.0382	0.025*	
C8	-0.01691 (10)	-0.2415 (3)	0.1459 (3)	0.0229 (6)	
H8A	-0.0158	-0.2989	0.0774	0.028*	
H8B	-0.0507	-0.2103	0.1418	0.028*	
C9	0	-0.3360 (4)	0.25	0.0267 (8)	
H9A	-0.0268	-0.3996	0.2614	0.032*	0.5
H9B	0.0268	-0.3996	0.2386	0.032*	0.5
C10	0.19091 (11)	-0.0047 (3)	-0.0660 (3)	0.0212 (6)	
C11	0.23991 (11)	0.0099 (3)	0.0154 (3)	0.0309 (7)	
H11A	0.2448	0.1116	0.0404	0.046*	
H11B	0.2656	-0.0191	-0.0229	0.046*	
H11C	0.2407	-0.0535	0.0807	0.046*	
C12	0.19012 (12)	0.0918 (4)	-0.1696 (3)	0.0329 (7)	
H12A	0.1592	0.0799	-0.2228	0.049*	
H12B	0.2164	0.0628	-0.2059	0.049*	
H12C	0.1943	0.1942	-0.1463	0.049*	
C13	0.18436 (12)	-0.1650 (3)	-0.1058 (3)	0.0321 (7)	
H13A	0.1883	-0.2296	-0.0402	0.048*	
H13B	0.2086	-0.1892	-0.1496	0.048*	
H13C	0.152	-0.1779	-0.1528	0.048*	
C14	0.11796 (9)	0.3942 (3)	0.1360 (3)	0.0235 (6)	
H14	0.1095	0.3925	0.2118	0.028*	
C15	0.17227 (12)	0.5804 (3)	0.2073 (3)	0.0339 (8)	
H15A	0.1503	0.6532	0.1651	0.051*	
H15B	0.2057	0.6133	0.2146	0.051*	

H15C	0.1652	0.5682	0.2824	0.051*
C16	0.09516 (15)	0.5158 (3)	-0.0422 (4)	0.0361 (8)
H16A	0.1253	0.5713	-0.033	0.054*
H16B	0.0688	0.5723	-0.088	0.054*
H16C	0.0986	0.4228	-0.0796	0.054*
N1	0.01452 (8)	-0.1109 (2)	0.1508 (2)	0.0204 (5)
O1	0.16587 (7)	0.4450 (2)	0.1494 (2)	0.0290 (5)
O2	0.08471 (8)	0.4884 (2)	0.0652 (2)	0.0311 (6)
Ni1	0	0.03581 (5)	0.25	0.01859 (15)
S1	0.03409 (3)	0.21315 (7)	0.17667 (7)	0.02433 (18)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0216 (12)	0.0109 (12)	0.0249 (14)	-0.0007 (9)	0.0108 (11)	-0.0012 (10)
C2	0.0242 (12)	0.0106 (12)	0.0270 (14)	-0.0027 (9)	0.0091 (11)	-0.0017 (10)
C3	0.0242 (13)	0.0124 (12)	0.0284 (15)	-0.0023 (9)	0.0112 (11)	0.0006 (10)
C4	0.0212 (12)	0.0131 (12)	0.0256 (15)	-0.0007 (9)	0.0079 (11)	0.0003 (10)
C5	0.0242 (13)	0.0100 (12)	0.0277 (15)	-0.0013 (9)	0.0097 (11)	-0.0009 (10)
C6	0.0190 (12)	0.0095 (12)	0.0304 (16)	-0.0023 (9)	0.0092 (11)	-0.0011 (10)
C7	0.0243 (12)	0.0131 (12)	0.0254 (15)	-0.0036 (10)	0.0059 (11)	-0.0036 (10)
C8	0.0266 (13)	0.0161 (13)	0.0278 (16)	-0.0069 (10)	0.0095 (12)	-0.0022 (11)
C9	0.038 (2)	0.0121 (18)	0.034 (2)	0	0.016 (2)	0
C10	0.0259 (13)	0.0098 (12)	0.0321 (17)	0.0013 (9)	0.0154 (13)	0.0008 (10)
C11	0.0229 (14)	0.0263 (16)	0.045 (2)	0.0031 (11)	0.0095 (15)	-0.0008 (13)
C12	0.0465 (17)	0.0230 (15)	0.0354 (19)	0.0070 (13)	0.0227 (15)	0.0074 (13)
C13	0.0380 (16)	0.0121 (14)	0.053 (2)	0.0002 (11)	0.0242 (15)	-0.0052 (12)
C14	0.0273 (13)	0.0126 (13)	0.0337 (17)	-0.0037 (10)	0.0131 (12)	-0.0053 (11)
C15	0.0441 (18)	0.0184 (15)	0.042 (2)	-0.0098 (12)	0.0160 (15)	-0.0142 (13)
C16	0.052 (2)	0.0176 (15)	0.036 (2)	-0.0112 (13)	0.0022 (17)	0.0011 (13)
N1	0.0237 (11)	0.0108 (10)	0.0268 (13)	-0.0035 (8)	0.0053 (9)	-0.0007 (9)
O1	0.0297 (11)	0.0162 (10)	0.0444 (14)	-0.0080 (8)	0.0153 (10)	-0.0127 (9)
O2	0.0354 (12)	0.0130 (10)	0.0465 (17)	0.0013 (8)	0.0121 (11)	-0.0008 (9)
Ni1	0.0206 (2)	0.0115 (2)	0.0264 (3)	0	0.0112 (2)	0
S1	0.0298 (3)	0.0120 (3)	0.0370 (4)	-0.0027 (2)	0.0204 (3)	-0.0034 (3)

*Geometric parameters (Å, °)*

C1—C6	1.418 (3)	C11—H11A	0.98
C1—C2	1.423 (4)	C11—H11B	0.98
C1—S1	1.749 (3)	C11—H11C	0.98
C2—C3	1.388 (4)	C12—H12A	0.98
C2—C14	1.527 (4)	C12—H12B	0.98
C3—C4	1.404 (4)	C12—H12C	0.98
C3—H3	0.95	C13—H13A	0.98
C4—C5	1.392 (4)	C13—H13B	0.98
C4—C10	1.535 (4)	C13—H13C	0.98
C5—C6	1.407 (4)	C14—O1	1.413 (3)

C5—H5	0.95	C14—O2	1.425 (4)
C6—C7	1.450 (4)	C14—H14	1
C7—N1	1.288 (4)	C15—O1	1.418 (3)
C7—H7	0.95	C15—H15A	0.98
C8—N1	1.485 (3)	C15—H15B	0.98
C8—C9	1.525 (4)	C15—H15C	0.98
C8—H8A	0.99	C16—O2	1.420 (5)
C8—H8B	0.99	C16—H16A	0.98
C9—C8 <sup>i</sup>	1.525 (4)	C16—H16B	0.98
C9—H9A	0.99	C16—H16C	0.98
C9—H9B	0.99	Ni1—N1	1.907 (2)
C10—C11	1.532 (5)	Ni1—N1 <sup>i</sup>	1.907 (2)
C10—C12	1.534 (4)	Ni1—S1 <sup>i</sup>	2.1742 (8)
C10—C13	1.543 (4)	Ni1—S1	2.1742 (8)
C6—C1—C2	116.6 (2)	H11B—C11—H11C	109.5
C6—C1—S1	124.08 (19)	C10—C12—H12A	109.5
C2—C1—S1	119.2 (2)	C10—C12—H12B	109.5
C3—C2—C1	120.9 (2)	H12A—C12—H12B	109.5
C3—C2—C14	120.2 (2)	C10—C12—H12C	109.5
C1—C2—C14	118.9 (2)	H12A—C12—H12C	109.5
C2—C3—C4	122.9 (2)	H12B—C12—H12C	109.5
C2—C3—H3	118.5	C10—C13—H13A	109.5
C4—C3—H3	118.5	C10—C13—H13B	109.5
C5—C4—C3	116.2 (3)	H13A—C13—H13B	109.5
C5—C4—C10	123.0 (2)	C10—C13—H13C	109.5
C3—C4—C10	120.8 (2)	H13A—C13—H13C	109.5
C4—C5—C6	122.6 (2)	H13B—C13—H13C	109.5
C4—C5—H5	118.7	O1—C14—O2	111.6 (2)
C6—C5—H5	118.7	O1—C14—C2	108.2 (2)
C5—C6—C1	120.7 (2)	O2—C14—C2	112.8 (2)
C5—C6—C7	115.1 (2)	O1—C14—H14	108.1
C1—C6—C7	124.2 (2)	O2—C14—H14	108.1
N1—C7—C6	127.8 (3)	C2—C14—H14	108.1
N1—C7—H7	116.1	O1—C15—H15A	109.5
C6—C7—H7	116.1	O1—C15—H15B	109.5
N1—C8—C9	110.0 (2)	H15A—C15—H15B	109.5
N1—C8—H8A	109.7	O1—C15—H15C	109.5
C9—C8—H8A	109.7	H15A—C15—H15C	109.5
N1—C8—H8B	109.7	H15B—C15—H15C	109.5
C9—C8—H8B	109.7	O2—C16—H16A	109.5
H8A—C8—H8B	108.2	O2—C16—H16B	109.5
C8 <sup>i</sup> —C9—C8	110.8 (3)	H16A—C16—H16B	109.5
C8 <sup>i</sup> —C9—H9A	109.5	O2—C16—H16C	109.5
C8—C9—H9A	109.5	H16A—C16—H16C	109.5
C8 <sup>i</sup> —C9—H9B	109.5	H16B—C16—H16C	109.5
C8—C9—H9B	109.5	C7—N1—C8	115.5 (2)
H9A—C9—H9B	108.1	C7—N1—Ni1	131.74 (19)

C11—C10—C12	109.5 (3)	C8—N1—Ni1	112.60 (18)
C11—C10—C4	108.8 (3)	C14—O1—C15	111.4 (2)
C12—C10—C4	109.6 (2)	C16—O2—C14	115.0 (3)
C11—C10—C13	108.5 (2)	N1—Ni1—N1 <sup>i</sup>	90.49 (14)
C12—C10—C13	108.1 (3)	N1—Ni1—S1 <sup>i</sup>	163.52 (7)
C4—C10—C13	112.3 (2)	N1 <sup>i</sup> —Ni1—S1 <sup>i</sup>	95.30 (7)
C10—C11—H11A	109.5	N1—Ni1—S1	95.30 (7)
C10—C11—H11B	109.5	N1 <sup>i</sup> —Ni1—S1	163.52 (7)
H11A—C11—H11B	109.5	S1 <sup>i</sup> —Ni1—S1	83.41 (4)
C10—C11—H11C	109.5	C1—S1—Ni1	109.86 (9)
H11A—C11—H11C	109.5		
C6—C1—C2—C3	-0.9 (4)	C3—C4—C10—C13	179.5 (3)
S1—C1—C2—C3	-178.0 (2)	C3—C2—C14—O1	-21.8 (4)
C6—C1—C2—C14	-178.9 (3)	C1—C2—C14—O1	156.3 (3)
S1—C1—C2—C14	3.9 (4)	C3—C2—C14—O2	102.1 (3)
C1—C2—C3—C4	2.6 (5)	C1—C2—C14—O2	-79.8 (3)
C14—C2—C3—C4	-179.4 (3)	C6—C7—N1—C8	180.0 (3)
C2—C3—C4—C5	-1.4 (4)	C6—C7—N1—Ni1	4.6 (5)
C2—C3—C4—C10	179.7 (3)	C9—C8—N1—C7	106.0 (3)
C3—C4—C5—C6	-1.4 (4)	C9—C8—N1—Ni1	-77.7 (2)
C10—C4—C5—C6	177.4 (3)	O2—C14—O1—C15	65.2 (3)
C4—C5—C6—C1	3.1 (5)	C2—C14—O1—C15	-170.2 (3)
C4—C5—C6—C7	-177.7 (3)	O1—C14—O2—C16	54.4 (3)
C2—C1—C6—C5	-1.8 (4)	C2—C14—O2—C16	-67.6 (3)
S1—C1—C6—C5	175.1 (2)	C7—N1—Ni1—N1 <sup>i</sup>	-149.1 (3)
C2—C1—C6—C7	179.0 (3)	C8—N1—Ni1—N1 <sup>i</sup>	35.38 (15)
S1—C1—C6—C7	-4.0 (4)	C7—N1—Ni1—S1 <sup>i</sup>	100.1 (3)
C5—C6—C7—N1	166.0 (3)	C8—N1—Ni1—S1 <sup>i</sup>	-75.4 (3)
C1—C6—C7—N1	-14.8 (5)	C7—N1—Ni1—S1	15.4 (3)
N1—C8—C9—C8 <sup>i</sup>	37.87 (15)	C8—N1—Ni1—S1	-160.07 (17)
C5—C4—C10—C11	-119.5 (3)	C6—C1—S1—Ni1	24.5 (3)
C3—C4—C10—C11	59.3 (3)	C2—C1—S1—Ni1	-158.6 (2)
C5—C4—C10—C12	120.8 (3)	N1—Ni1—S1—C1	-24.99 (12)
C3—C4—C10—C12	-60.4 (4)	N1 <sup>i</sup> —Ni1—S1—C1	85.1 (3)
C5—C4—C10—C13	0.6 (4)	S1 <sup>i</sup> —Ni1—S1—C1	171.52 (11)

Symmetry code: (i)  $-x, y, -z+1/2$ .