

Retraction of articles

This article reports the retraction of 39 articles published in *Acta Crystallographica Section E* between 2004 and 2009.

After thorough investigation (see Harrison *et al.*, 2010), 39 additional articles are retracted as a result of problems with the data sets or incorrect atom assignments. Full details of all the articles are given in Table 1.

Table 1

Details of articles to be retracted, in order of publication.

Title	Reference	Retracted by	DOI	Refcode
<i>trans</i> -Bis[1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato]copper(II) dichloride dihydrate	Zhang (2004)	Journal	10.1107/S1600536804028296	BIPDUA
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$)copper(II)	Sun & Gao (2005)	Author	10.1107/S160053680500187X	FEYSUY
Bis(salicylaldehyde)zinc(II)	Xiong & Liu (2005)	Journal	10.1107/S1600536805010913	GAMDUU
Bis(4-bromo-2-formylphenolato- $\kappa^2 O, O'$)zinc(II)	Chen (2006)	Journal	10.1107/S1600536805040432	SAZCUS
Bis(2-formylphenolato- $\kappa^2 O, O'$)nickel(II)	Li & Chen (2006)	Journal	10.1107/S1600536806012931	IDAZAP
Bis(2-formylphenolato)cobalt(II)	Qiu (2006)	Journal	10.1107/S1600536806015704	GEJDUV
Bis(2-formylphenolato- $\kappa^2 O, O'$)manganese(II)	Wang & Fang (2006)	Journal	10.1107/S1600536806021039	IDOVED
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)copper(II) naphthalene-1,5-disulfonate dihydrate	Liu <i>et al.</i> (2006)	Author	10.1107/S1600536806030637	GENYOO
Tetraaqua(1,10-phenanthroline- $\kappa^2 N, N'$)nickel(II) naphthalene-1,5-disulfonate dihydrate	Liu & Fan (2006)	Author	10.1107/S1600536806035410	KERBEP
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratolutetium(III)copper(II)	Sui <i>et al.</i> (2006)	Journal	10.1107/S160053680604565X	HESPEB
Bis(2-formylphenolato- $\kappa^2 O, O'$)iron(II)	Yang <i>et al.</i> (2007)	Author	10.1107/S1600536807021721	PIFCAJ
2,6-Dimethoxybenzohydrazide	Qadeer <i>et al.</i> (2007a)	Journal	10.1107/S1600536807022593	PIFHES
2-(2,4-Dichlorophenylsulfanyl)acetohydrazide	Qadeer <i>et al.</i> (2007b)	Journal	10.1107/S1600536807022891	YIFSOW
{6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2007)	Author	10.1107/S1600536807031121	WIHKEE
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratocerium(III)zinc(II)	Sui, Zhang, Hu & Yin (2007)	Author	10.1107/S1600536807032564	WIHREL
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)zinc(II)	Chen <i>et al.</i> (2007)	Author	10.1107/S1600536807032540	WIHRIP
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)	Sui, Li <i>et al.</i> (2007)	Author	10.1107/S1600536807032618	UFACUA
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1 $\kappa^4 O^1, O^2, O^3, O^4, O^5, O^6, O^7, O^8, O^9, O^{10}$:2 $\kappa^2 O^1, N, N', N'', N'''$ }(methanol-1 κO)- μ -nitrate-1:2 $\kappa^2 O:O'$ -dinitrate-1 $\kappa^4 O, O'$ -cerium(III)zinc(II)	Sui, Fang, Hu & Lin (2007)	Author	10.1107/S1600536807033314	UDUYIC
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol- μ -nitrate-dinitratosamarium(III)nickel(II)	Sui, Zhang, Hu & Jiang (2007)	Author	10.1107/S1600536807037130	AFECEU
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol- μ -nitrate-dinitratopraseodymium(III)zinc(II)	Sui, Fang & Yuan (2007)	Author	10.1107/S1600536807037488	AFICEY
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-methanol- μ -nitrate-dinitratolutetium(III)zinc(II)	Sui, Sui <i>et al.</i> (2007)	Author	10.1107/S1600536807037737	AFEF0H
catena-Poly[[chloridonickel(II)]-di- μ -chlorido-[chloridonickel(II)]- μ -4,4'-methylenebis(3,5-dimethylpyrazole)- $\kappa^2 N^2, N^2$]	Huang & Chen (2007)	Author	10.1107/S1600536807039384	VIJYOD
[2,2'-[<i>o</i> -Phenylenebis(nitrilomethylidyne)]diphenolato]zinc(II)	Liu <i>et al.</i> (2007a)	Author	10.1107/S1600536807040640	DIKYUS
<i>trans</i> -Bis(ethylenediamine- $\kappa^2 N, N'$)bis(nitrate- κO)zinc(II)	Liu, Zeng & Chen (2007)	Author	10.1107/S1600536807042390	XIKYEW
[<i>N, N'</i> -(<i>o</i> -Phenylene)bis(picolinamido)- $\kappa^2 N, N', N'', N'''$]cobalt(II)	Liu & Zeng (2007a)	Author	10.1107/S1600536807044571	XILFII
[<i>N, N'</i> -(<i>o</i> -Phenylene)dipicolinamide- $\kappa^2 N$]nickel(II)	Liu & Zeng (2007b)	Author	10.1107/S1600536807048386	WINWEW
[2,2'-[<i>o</i> -Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)	Liu <i>et al.</i> (2007b)	Author	10.1107/S1600536807052993	VIQPIV
<i>N</i> -(2-Amino-3-pyridyl)urea monohydrate	Li <i>et al.</i> (2007)	Author	10.1107/S1600536807047526	SIMFEA
<i>N</i> -(2-Fluorophenyl)carbamic acid monohydrate	Yang (2007)	Author	10.1107/S1600536807052464	WINMOW
Aqua(dimethylglyoxime- $\kappa^2 N, N'$)(3,5-dinitro-2-oxidobenzooato- $\kappa^2 O^1, O^2$)-copper(II)	Liu & Wen (2007)	Author	10.1107/S1600536807054244	HIQCAM
μ -Acetato-tri- μ -ferrocenecarboxylatobis[(<i>N, N</i> -dimethylformamide)-copper(II)]	Liu, Lin <i>et al.</i> (2007)	Journal	10.1107/S1600536807059041	HIQQEE

Table 1 (continued)

Title	Reference	Retracted by	DOI	Refcode
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoeuropium(III)zinc(II)	Hu <i>et al.</i> (2008)	Author	10.1107/S160053680706151X	MIRPAF
Bis(4-chloro-2-formylphenolato)nickel(II)	Li <i>et al.</i> (2008)	Author	10.1107/S1600536807056309	RISTET
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoerbium(III)zinc(II)	Chen <i>et al.</i> (2008)	Author	10.1107/S1600536808006958	QIXHIP
Bis(2-ethoxy-6-formylphenolato- $\kappa^2 O^1, O^6$)nickel(II)	Han (2008)	Journal	10.1107/S160053680800809X	QIXLIT
{ μ -6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}- μ -nitrate-dinitratoholmium(III)zinc(II)	Xiao, Sui <i>et al.</i> (2008)	Author	10.1107/S1600536808013743	BIZTUA
{ μ -6,6'-Diethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoholmium(III)nickel(II)	Xiao, Fu <i>et al.</i> (2008)	Author	10.1107/S1600536808013755	BIZVAI
Hydrogen-bonding patterns in the cocrystal terephthalic acid-4,4'-bipyridine (2I)	Wang <i>et al.</i> (2009)	Journal	10.1107/S160053680903236X	DUCZEH
{6,6'-Dimethoxy-2,2'-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1 $\kappa^4 O^1, O^1, O^6, O^6$:2 $\kappa^4 O^1, N, N, O^1$ } (ethanol-1 κO)- μ -nitrate-1:2 $\kappa^2 O: O'$ -dinitrate-1 $\kappa^2 O, O'$ -samarium(III)zinc(II)	Huang <i>et al.</i> (2009)	Journal	10.1107/S1600536809033558	YUCWAV

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Bis(4-chloro-2-formylphenolato)-nickel(II)

Zongxiao Li,* Xinli Zhang and Xiaohua Pu

Department of Chemistry, Baoji University of Arts and Science, Baoji, Shaanxi 721007, People's Republic of China

Correspondence e-mail: mingtian8001@163.com

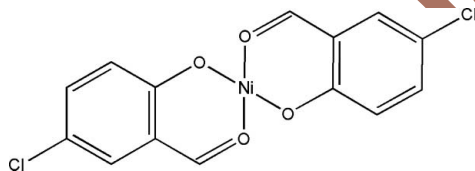
Received 5 November 2007; accepted 6 November 2007

Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.034; wR factor = 0.093; data-to-parameter ratio = 12.9.

The asymmetric unit of the title compound, $[\text{Ni}(\text{C}_7\text{H}_4\text{ClO}_2)_2]$, contains one half-molecule. The Ni^{II} ion, lying on an inversion centre, is four-coordinated by O atoms of 5-chlorosalicylaldehyde ligands in a square-planar geometry.

Related literature

For general background, see: Gavrilova & Bosnich (2004); Boudalis *et al.* (2004); Veauthier *et al.* (2004). For related structures, see: Erxleben *et al.* (2001). For bond-length data, see: Allen *et al.* 1987.



Experimental

Crystal data

$[\text{Ni}(\text{C}_7\text{H}_4\text{ClO}_2)_2]$
 $M_r = 369.81$
 Monoclinic, $P2_1/c$
 $a = 15.765$ (3) Å
 $b = 5.6921$ (14) Å
 $c = 7.8869$ (14) Å

$\beta = 93.896$ (2)°
 $V = 706.1$ (3) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.76$ mm⁻¹
 $T = 298$ (2) K

$0.20 \times 0.17 \times 0.12$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\text{min}} = 0.720$, $T_{\text{max}} = 0.816$
 3455 measured reflections
 1250 independent reflections
 1056 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.034$
 $wR(F^2) = 0.093$
 $S = 1.10$
 1250 reflections
 97 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.55$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.43$ e Å⁻³

Table 1

Selected geometric parameters (Å, °)

Ni1—O2	1.840 (2)	Ni1—O1	1.851 (3)
O2 ⁱ —Ni1—O2	180	O2—Ni1—O1	94.40 (10)
O2 ⁱ —Ni1—O1	85.60 (10)	O1—Ni1—O1 ⁱ	180

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

Data collection: SMART (Bruker, 1997); cell refinement: SAINT (Bruker, 1997); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 1995); software used to prepare material for publication: SHELXTL.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2368).

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supporting information

Acta Cryst. (2008). E64, m215 [https://doi.org/10.1107/S1600536807056309]

Bis(4-chloro-2-formylphenolato)nickel(II)

Zongxiao Li, Xinli Zhang and Xiaohua Pu

S1. Comment

The design of multidentate ligands and their metallosupramolecular chemistry are of great interest in the last few years (Gavrilova & Bosnich, 2004; Boudalis *et al.*, 2004; Veauthier *et al.*, 2004). As an extension of our ongoing studies on the structural characterization of Schiff base compounds, we report herein the crystal structure of the title compound, (I).

The asymmetric unit of (I) contains one-half molecule (Fig. 1), in which the bond lengths and angles (Table 1) are within normal ranges (Allen *et al.*, 1987). It is a mononuclear Ni^{II} complex being structurally similar to the Co(II) and Zn(II) complexes derived from other Schiff base ligands (Erxleben *et al.*, 2001). The Ni^{II} ion is four-coordinated by symmetry-related O atoms of 5-chlorosalicylaldehydato ligands.

S2. Experimental

For the preparation of the title compound, (I), 5-chlorosalicylaldehyde (15.7 mg, 0.1 mmol) and Ni(NO₃)₂·6(H₂O) (29.0 mg, 0.1 mmol) were dissolved in methanol (10 ml). The mixture was stirred for 30 min at room temperature to give a clear brown solution. After allowing the resulting solution to stand in air for 11 d, brown block-shaped crystals of (I) were formed by slow evaporation of the solvent. The crystals were collected, washed with methanol and dried in a vacuum desiccator using anhydrous CaCl₂ (yield; 54%). Elemental analysis; found C 45.42%, H 2.16%; calc. for C₁₄H₈Cl₂Ni O₄: C 45.44, H 2.61%.

S3. Refinement

H atoms were positioned geometrically, with C—H = 0.93 Å, for aromatic H atoms and constrained to ride on their parent atoms, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

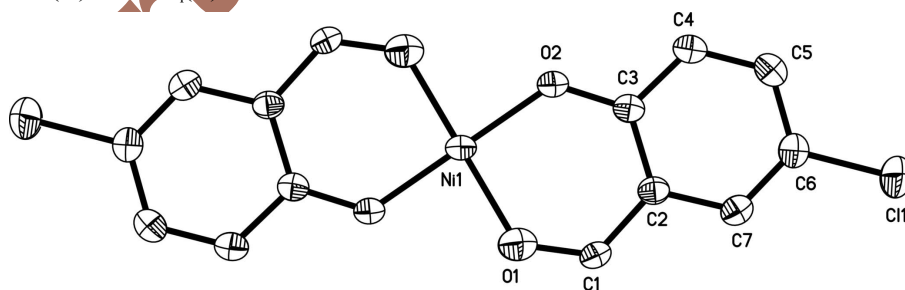


Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Bis(4-chloro-2-formylphenolato)nickel(II)

Crystal data

[Ni(C₇H₄ClO₂)₂] $M_r = 369.81$ Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

 $a = 15.765 (3) \text{ \AA}$ $b = 5.6921 (14) \text{ \AA}$ $c = 7.8869 (14) \text{ \AA}$ $\beta = 93.896 (2)^\circ$ $V = 706.1 (3) \text{ \AA}^3$ $Z = 2$ $F(000) = 372$ $D_x = 1.739 \text{ Mg m}^{-3}$ Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 1788 reflections

 $\theta = 2.6\text{--}27.2^\circ$ $\mu = 1.76 \text{ mm}^{-1}$ $T = 298 \text{ K}$

Block, brown

 $0.20 \times 0.17 \times 0.12 \text{ mm}$

Data collection

Bruker SMART CCD area-detector

diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

 φ and ω scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

 $T_{\min} = 0.720$, $T_{\max} = 0.816$

3455 measured reflections

1250 independent reflections

1056 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.019$ $\theta_{\max} = 25.0^\circ$, $\theta_{\min} = 2.6^\circ$ $h = -18 \rightarrow 15$ $k = -6 \rightarrow 6$ $l = -7 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

 $R[F^2 > 2\sigma(F^2)] = 0.034$ $wR(F^2) = 0.093$ $S = 1.10$

1250 reflections

97 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

 $w = 1/[\sigma^2(F_o^2) + (0.0455P)^2 + 0.5565P]$ where $P = (F_o^2 + 2F_c^2)/3$ $(\Delta/\sigma)_{\max} < 0.001$ $\Delta\rho_{\max} = 0.55 \text{ e \AA}^{-3}$ $\Delta\rho_{\min} = -0.43 \text{ e \AA}^{-3}$

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)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.5000	0.0000	0.0000	0.0368 (2)
Cl1	0.06478 (6)	0.1508 (2)	0.19360 (16)	0.0813 (4)
O1	0.45925 (17)	0.2599 (5)	0.1098 (3)	0.0634 (7)
O2	0.39686 (13)	-0.1524 (3)	-0.0165 (3)	0.0434 (5)

C1	0.3822 (2)	0.3016 (5)	0.1485 (4)	0.0425 (7)
H1	0.3714	0.4431	0.2018	0.051*
C2	0.3126 (2)	0.1431 (5)	0.1141 (4)	0.0398 (7)
C3	0.32369 (19)	-0.0744 (6)	0.0312 (4)	0.0389 (7)
C4	0.2507 (2)	-0.2141 (6)	-0.0042 (4)	0.0465 (8)
H4	0.2557	-0.3559	-0.0613	0.056*
C5	0.1722 (2)	-0.1449 (6)	0.0438 (5)	0.0528 (9)
H5	0.1250	-0.2402	0.0197	0.063*
C6	0.1633 (2)	0.0666 (7)	0.1281 (4)	0.0497 (8)
C7	0.2316 (2)	0.2091 (6)	0.1627 (4)	0.0460 (8)
H7	0.2248	0.3508	0.2189	0.055*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0449 (3)	0.0309 (3)	0.0342 (3)	-0.0012 (2)	0.0001 (2)	-0.0031 (2)
Cl1	0.0502 (6)	0.0935 (9)	0.1021 (9)	0.0018 (5)	0.0186 (5)	-0.0168 (7)
O1	0.0725 (18)	0.0565 (15)	0.0609 (16)	-0.0023 (13)	0.0037 (13)	-0.0085 (13)
O2	0.0464 (12)	0.0340 (11)	0.0499 (13)	-0.0011 (9)	0.0035 (10)	-0.0066 (10)
C1	0.0490 (19)	0.0354 (16)	0.0433 (18)	0.0045 (14)	0.0057 (14)	-0.0065 (14)
C2	0.0469 (17)	0.0353 (17)	0.0369 (16)	0.0006 (13)	0.0008 (13)	0.0006 (13)
C3	0.0461 (18)	0.0350 (15)	0.0351 (16)	-0.0009 (13)	-0.0004 (13)	0.0037 (13)
C4	0.054 (2)	0.0388 (17)	0.0462 (19)	-0.0042 (14)	0.0003 (15)	-0.0023 (14)
C5	0.0481 (19)	0.053 (2)	0.056 (2)	-0.0091 (16)	0.0002 (16)	0.0002 (17)
C6	0.0443 (18)	0.055 (2)	0.050 (2)	0.0024 (15)	0.0048 (15)	0.0025 (16)
C7	0.0518 (19)	0.0422 (18)	0.0441 (19)	0.0056 (15)	0.0046 (15)	-0.0015 (14)

Geometric parameters (\AA , $^\circ$)

Ni1—O2 ⁱ	1.840 (2)	C2—C7	1.408 (4)
Ni1—O2	1.840 (2)	C2—C3	1.417 (4)
Ni1—O1	1.851 (3)	C3—C4	1.411 (4)
Ni1—O1 ⁱ	1.851 (3)	C4—C5	1.376 (5)
Cl1—C6	1.738 (3)	C4—H4	0.9300
O1—C1	1.294 (4)	C5—C6	1.387 (5)
O2—C3	1.315 (4)	C5—H5	0.9300
C1—C2	1.433 (4)	C6—C7	1.361 (5)
C1—H1	0.9300	C7—H7	0.9300
O2 ⁱ —Ni1—O2	180	O2—C3—C2	124.5 (3)
O2 ⁱ —Ni1—O1	85.60 (10)	C4—C3—C2	117.3 (3)
O2—Ni1—O1	94.40 (10)	C5—C4—C3	121.4 (3)
O2 ⁱ —Ni1—O1 ⁱ	94.40 (10)	C5—C4—H4	119.3
O2—Ni1—O1 ⁱ	85.60 (10)	C3—C4—H4	119.3
O1—Ni1—O1 ⁱ	180	C4—C5—C6	120.2 (3)
C1—O1—Ni1	128.2 (2)	C4—C5—H5	119.9
C3—O2—Ni1	127.52 (19)	C6—C5—H5	119.9
O1—C1—C2	124.0 (3)	C7—C6—C5	120.6 (3)

O1—C1—H1	118.0	C7—C6—C11	119.1 (3)
C2—C1—H1	118.0	C5—C6—C11	120.2 (3)
C7—C2—C3	120.1 (3)	C6—C7—C2	120.4 (3)
C7—C2—C1	118.5 (3)	C6—C7—H7	119.8
C3—C2—C1	121.3 (3)	C2—C7—H7	119.8
O2—C3—C4	118.2 (3)		
O2 ⁱ —Ni1—O1—C1	177.8 (3)	C7—C2—C3—C4	2.0 (4)
O2—Ni1—O1—C1	-2.2 (3)	C1—C2—C3—C4	-177.2 (3)
O1—Ni1—O2—C3	3.1 (3)	O2—C3—C4—C5	179.2 (3)
O1 ⁱ —Ni1—O2—C3	-176.9 (3)	C2—C3—C4—C5	-1.7 (5)
Ni1—O1—C1—C2	1.5 (5)	C3—C4—C5—C6	0.4 (5)
O1—C1—C2—C7	179.9 (3)	C4—C5—C6—C7	0.6 (5)
O1—C1—C2—C3	-0.8 (5)	C4—C5—C6—C11	-178.4 (3)
Ni1—O2—C3—C4	175.5 (2)	C5—C6—C7—C2	-0.3 (5)
Ni1—O2—C3—C2	-3.5 (4)	C11—C6—C7—C2	178.7 (2)
C7—C2—C3—O2	-178.9 (3)	C3—C2—C7—C6	-1.1 (5)
C1—C2—C3—O2	1.9 (5)	C1—C2—C7—C6	178.1 (3)

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

Article retracted