

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 $\kappa^2 O:O'$ -dinitrato-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'-[o-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
[N, N' -(<i>o</i> -Phenylene)bis(picolinamido)- $\kappa^2 N, N', N'', N'''$]cobalt(II)	Liu & Zeng (2007a)	Author	10.1107/S1600536807044571	XILFII
[N, N' -(<i>o</i> -Phenylene)dipicolinamide- $\kappa^2 N$]nickel(II)	Liu & Zeng (2007b)	Author	10.1107/S1600536807048386	WINWEW
[2,2'-[o-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'-dinitrato-1 $\kappa^4 O, O'$ -samarium(III)zinc(II)	Huang <i>et al.</i> (2009)	Journal	10.1107/S1600536809033558	YUCWAV

References

- Chen, Q. (2006). *Acta Cryst.* **E62**, m56–m57.
- Chen, J.-R., Sui, Y., Luo, Q.-Y. & Jiang, R.-Q. (2007). *Acta Cryst.* **E63**, m2091–m2092.
- Chen, J.-R., Sui, Y., Chen, L., Wen, J.-W. & Yin, L.-Y. (2008). *Acta Cryst.* **E64**, m562–m563.
- Han, Z.-Q. (2008). *Acta Cryst.* **E64**, m592.
- Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* **E66**, e1–e2.
- Hu, R.-H., Sui, Y., Chen, L. & He, C.-M. (2008). *Acta Cryst.* **E64**, m8–m9.
- Hu, R.-H., Sui, Y., Fang, X.-N. & Chen, H.-M. (2007). *Acta Cryst.* **E63**, m2039–m2040.
- Huang, C.-F. & Chen, H.-L. (2007). *Acta Cryst.* **E63**, m2356–m2357.
- Huang, Q., Sui, Y.-H. & Zhang, G.-X. (2009). *Acta Cryst.* **E65**, m1161–m1162.
- Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* **E62**, m1038–m1039.
- Li, N.-G., Tao, R.-M. & Fu, B.-F. (2007). *Acta Cryst.* **E63**, o4228.
- Li, Z., Zhang, X. & Pu, X. (2008). *Acta Cryst.* **E64**, m215.
- Liu, J.-T. & Fan, S.-D. (2006). *Acta Cryst.* **E62**, m2507–m2508.
- Liu, J.-T., Fan, S.-D. & Li, D.-Q. (2006). *Acta Cryst.* **E62**, m2165–m2166.
- Liu, D., Lin, J., Xu, Y., Huang, C. & Li, X. (2007). *Acta Cryst.* **E63**, m3094.
- Liu, Y.-Q. & Wen, H.-R. (2007). *Acta Cryst.* **E63**, m2928.
- Liu, Y.-Q. & Zeng, X.-R. (2007a). *Acta Cryst.* **E63**, m2547.
- Liu, Y.-Q. & Zeng, X.-R. (2007b). *Acta Cryst.* **E63**, m2684.
- Liu, Y.-Q., Zeng, X.-R. & Chen, W.-T. (2007). *Acta Cryst.* **E63**, m2462.
- Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007a). *Acta Cryst.* **E63**, m2396.
- Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007b). *Acta Cryst.* **E63**, m2854.
- Qadeer, G., Rama, N. H. & Chen, W.-T. (2007a). *Acta Cryst.* **E63**, o2892.
- Qadeer, G., Rama, N. H. & Chen, W.-T. (2007b). *Acta Cryst.* **E63**, o2932.
- Qiu, X.-Y. (2006). *Acta Cryst.* **E62**, m1190–m1191.
- Sui, Y., Fang, X.-N., Hu, P. & Lin, J. (2007). *Acta Cryst.* **E63**, m2135–m2136.
- Sui, Y., Fang, X.-N. & Yuan, M.-W. (2007). *Acta Cryst.* **E63**, m2275–m2276.
- Sui, Y., Li, X.-F., Huang, G.-S. & Wang, G.-J. (2007). *Acta Cryst.* **E63**, m2093–m2094.
- Sui, Y., Sui, Y.-H., Luo, Q.-Y. & Wang, Y.-D. (2007). *Acta Cryst.* **E63**, m2277–m2278.
- Sui, Y., Xiao, Y.-A., Fang, X.-N., Zeng, X.-R. & Li, M.-H. (2006). *Acta Cryst.* **E62**, m3205–m3207.
- Sui, Y., Zhang, J.-H., Hu, R.-H. & Jiang, R.-Q. (2007). *Acta Cryst.* **E63**, m2256–m2257.
- Sui, Y., Zhang, J.-H., Hu, R.-H. & Yin, L.-Y. (2007). *Acta Cryst.* **E63**, m2089–m2090.
- Sun, Y.-X. & Gao, G.-Z. (2005). *Acta Cryst.* **E61**, m354–m355.
- Wang, Q. & Fang, X.-N. (2006). *Acta Cryst.* **E62**, m1492–m1493.
- Wang, S., Yang, T., Li, Z. & Yu, X. (2009). *Acta Cryst.* **E65**, o2198.
- Xiao, Y.-A., Fu, X.-K., Sui, Y., Wu, Q. & Xiong, S.-H. (2008). *Acta Cryst.* **E64**, m806–m807.
- Xiao, Y.-A., Sui, Y., Yi, X.-G., Wu, J.-H. & Zhang, L.-P. (2008). *Acta Cryst.* **E64**, m804–m805.
- Xiong, Z.-Y. & Liu, L.-J. (2005). *Acta Cryst.* **E61**, m863–m864.
- Yang, X.-M. (2007). *Acta Cryst.* **E63**, o4453.
- Yang, Y.-M., Lu, P.-C., Zhu, T.-T. & Liu, C.-H. (2007). *Acta Cryst.* **E63**, m1613.
- Zhang, P. (2004). *Acta Cryst.* **E60**, m1808–m1810.

Bis(2-ethoxy-6-formylphenolato- κ^2O^1,O^6)nickel(II)

Zhen-Quan Han

Applied Technical College, Qiqihar University, Qiqihar 161006, People's Republic of China

Correspondence e-mail: zhenquan_han@126.com

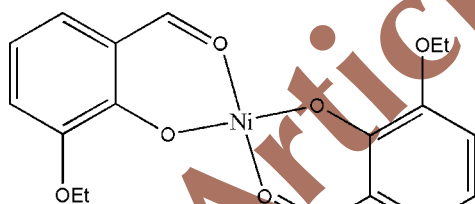
Received 18 March 2008; accepted 25 March 2008

 Key indicators: single-crystal X-ray study; $T = 298$ K; mean $\sigma(C-C) = 0.005$ Å; R factor = 0.042; wR factor = 0.116; data-to-parameter ratio = 17.3.

The title compound, $[Ni(C_9H_9O_3)_2]$, was synthesized by the reaction of 3-ethoxysalicylaldehyde with nickel(II) nitrate in methanol solution. The asymmetric unit consists of two half-molecules; each Ni atom lies on a centre of symmetry. The Ni^{II} ions are coordinated by four O atoms from two deprotonated 3-ethoxysalicylaldehyde ligands in a slightly distorted square-planar coordination environment.

Related literature

For related literature, see: Carlsson *et al.* (2004); Li & Chen (2006); Mounts & Fernando (1974); Volkmer *et al.* (1996).



Experimental

Crystal data

$[Ni(C_9H_9O_3)_2]$
 $M_r = 389.03$
 Triclinic, $P\bar{1}$
 $a = 8.448$ (2) Å

$b = 10.123$ (2) Å
 $c = 11.919$ (3) Å
 $\alpha = 111.175$ (2)°
 $\beta = 97.377$ (2)°

$\gamma = 102.431$ (3)°
 $V = 904.1$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation

$\mu = 1.10$ mm⁻¹
 $T = 298$ (2) K
 $0.32 \times 0.32 \times 0.30$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{min} = 0.719$, $T_{max} = 0.733$
 5465 measured reflections
 3993 independent reflections
 3187 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.013$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.116$
 $S = 1.02$
 3993 reflections
 231 parameters
 H-atom parameters constrained
 $\Delta\rho_{max} = 0.65$ e Å⁻³
 $\Delta\rho_{min} = -0.66$ e Å⁻³

Table 1

Selected geometric parameters (Å, °).

Ni1—O5	1.837 (2)	Ni2—O1	1.843 (2)
Ni1—O4	1.852 (2)	Ni2—O2	1.851 (2)
O5—Ni1—O5 ⁱ	180	O1—Ni2—O1 ⁱⁱ	180
O5—Ni1—O4	94.16 (9)	O1—Ni2—O2	93.70 (9)
O5 ⁱ —Ni1—O4	85.84 (9)	O1 ⁱⁱ —Ni2—O2	86.30 (9)
O4—Ni1—O4 ⁱ	180	O2 ⁱⁱ —Ni2—O2	180

 Symmetry codes: (i) $-x, -y + 1, -z$; (ii) $-x, -y, -z$.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

The author acknowledges Qiqihar University for a research grant.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2604).

References

- Bruker (1998). SMART (Version 5.628) and SAINT (Version 6.02). Bruker AXS Inc., Madison, Wisconsin, USA.
 Carlsson, H., Haukka, M., Bousseksou, A., Latour, J.-M. & Nordlander, E. (2004). *Inorg. Chem.* **43**, 8252–8262.
 Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* **E62**, m1038–m1039.
 Mounts, R. D. & Fernando, Q. (1974). *Acta Cryst.* **B30**, 542–543.
 Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Volkmer, D., Hommerich, B., Griesar, K., Haase, W. & Krebs, B. (1996). *Inorg. Chem.* **35**, 3792–3803.

supplementary materials

Article retracted

Acta Cryst. (2008). E64, m592 [doi:10.1107/S160053680800809X]

Bis(2-ethoxy-6-formylphenolato- κ^2O^1,O^6)nickel(II)

Z.-Q. Han

Comment

The authors interest in nickel(II) complexes arises from the fact that Ni(II) is the active center of the urease enzyme (Carlsson *et al.*, 2004; Volkmer *et al.*, 1996). The author reports herein the crystal structure of the title nickel(II) complex.

In the asymmetric unit of the title compound, there are two independent complex (Fig. 1). Each Ni^{II} ion lies on an inversion center and is coordinated by four O atoms from two deprotonated 3-ethoxysalicylaldehyde ligands. The coordinate bond values (Table 1) in each molecule are comparable to each other between the two independent complex molecules. The structure is similar to other nickel(II) complexes derived from the derivatives of salicylaldehyde (Li & Chen, 2006; Mounts & Fernando, 1974).

Experimental

All chemicals were of AR grade. 3-Ethoxysalicylaldehyde (33.2 mg, 0.2 mmol) and nickel(II) nitrate hexahydrate (29.0 mg, 0.1 mmol) were refluxed for 30 min in 10 ml methanol solution. The mixture was cooled to room temperature and filtered. Keeping the filtrate in air for a week, yielded red block crystals suitable for X-ray analysis.

Refinement

H atoms were placed in idealized positions and constrained to ride on their parent atoms with C–H distances in the range 0.93–0.97 Å, and with $U_{\text{iso}}(\text{H})$ set at $1.2U_{\text{eq}}(\text{C})$ and $1.5U_{\text{eq}}(\text{methyl C})$. Although no significant density was located in the solvent accessible VOIDS of 47.00 \AA^3 , these might be able to accommodate disordered water molecules.

Figures

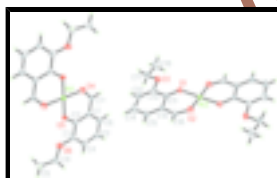


Fig. 1. The molecular structures of the two centrosymmetric independent molecules, showing 30% probability displacement ellipsoids and the atom-numbering scheme. The unlabeled atoms are related by the symmetry operators $(-x, -y+1, -z)$ and $(-x, -y, -z)$ for the molecules containing Ni1 and Ni2 respectively.

Bis(2-ethoxy-6-formylphenolato- κ^2O^1,O^6)nickel(II)

Crystal data

$[\text{Ni}(\text{C}_9\text{H}_9\text{O}_3)_2]$

$M_r = 389.03$

$Z = 2$

$F_{000} = 404$

supplementary materials

Triclinic, $P\bar{1}$	$D_x = 1.429 \text{ Mg m}^{-3}$
Hall symbol: -P 1	Mo $K\alpha$ radiation
$a = 8.448 (2) \text{ \AA}$	$\lambda = 0.71073 \text{ \AA}$
$b = 10.123 (2) \text{ \AA}$	Cell parameters from 2386 reflections
$c = 11.919 (3) \text{ \AA}$	$\theta = 2.2\text{--}27.9^\circ$
$\alpha = 111.175 (2)^\circ$	$\mu = 1.10 \text{ mm}^{-1}$
$\beta = 97.377 (2)^\circ$	$T = 298 (2) \text{ K}$
$\gamma = 102.431 (3)^\circ$	Block, red
$V = 904.1 (4) \text{ \AA}^3$	$0.32 \times 0.32 \times 0.30 \text{ mm}$

Data collection

Bruker SMART CCD area-detector diffractometer	3993 independent reflections
Radiation source: fine-focus sealed tube	3187 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{\text{int}} = 0.013$
$T = 298(2) \text{ K}$	$\theta_{\text{max}} = 27.5^\circ$
ω scans	$\theta_{\text{min}} = 2.3^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 8$
$T_{\text{min}} = 0.719$, $T_{\text{max}} = 0.733$	$k = -13 \rightarrow 13$
5465 measured reflections	$l = -11 \rightarrow 15$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H-atom parameters constrained
$wR(F^2) = 0.116$	$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.672P]$
$S = 1.02$	where $P = (F_o^2 + 2F_c^2)/3$
3993 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
231 parameters	$\Delta\rho_{\text{max}} = 0.65 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.66 \text{ e \AA}^{-3}$
	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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Ni1	0.0000	0.5000	0.0000	0.02805 (13)
Ni2	0.0000	0.0000	0.0000	0.02920 (14)
O1	0.0505 (2)	-0.0121 (2)	0.15045 (16)	0.0363 (4)
O2	-0.0576 (3)	0.1741 (2)	0.0663 (2)	0.0506 (5)
O3	0.1596 (3)	-0.0689 (2)	0.33683 (18)	0.0484 (5)
O4	0.0529 (3)	0.3494 (3)	-0.1190 (2)	0.0513 (5)
O5	0.1989 (2)	0.63719 (19)	0.02863 (17)	0.0350 (4)
O6	0.4541 (3)	0.8659 (2)	0.1053 (2)	0.0552 (6)
C1	0.3232 (3)	0.4873 (3)	-0.1220 (3)	0.0366 (6)
C2	0.3219 (3)	0.6192 (3)	-0.0278 (2)	0.0328 (5)
C3	0.4641 (3)	0.7438 (3)	0.0107 (3)	0.0416 (7)
C4	0.5959 (4)	0.7345 (4)	-0.0462 (3)	0.0534 (8)
H4	0.6872	0.8170	-0.0214	0.064*
C5	0.5940 (4)	0.6031 (4)	-0.1404 (3)	0.0583 (9)
H5	0.6837	0.5983	-0.1779	0.070*
C6	0.4608 (4)	0.4814 (4)	-0.1777 (3)	0.0508 (8)
H6	0.4606	0.3938	-0.2403	0.061*
C7	0.1866 (3)	0.3570 (3)	-0.1613 (3)	0.0387 (6)
H7	0.1946	0.2713	-0.2220	0.046*
C8	0.5934 (4)	0.9930 (4)	0.1562 (4)	0.0630 (10)
H8A	0.6162	1.0304	0.0939	0.076*
H8B	0.6910	0.9687	0.1859	0.076*
C9	0.5528 (5)	1.1062 (5)	0.2603 (4)	0.0745 (11)
H9A	0.4523	1.1251	0.2308	0.112*
H9B	0.6424	1.1959	0.2933	0.112*
H9C	0.5375	1.0706	0.3238	0.112*
C10	0.0426 (4)	0.2306 (3)	0.2817 (3)	0.0403 (6)
C11	0.0741 (3)	0.0937 (3)	0.2595 (2)	0.0344 (6)
C12	0.1373 (4)	0.0681 (3)	0.3646 (3)	0.0408 (6)
C13	0.1716 (5)	0.1762 (4)	0.4812 (3)	0.0603 (9)
H13	0.2143	0.1582	0.5484	0.072*
C14	0.1433 (6)	0.3135 (4)	0.5010 (3)	0.0737 (12)
H14	0.1689	0.3866	0.5806	0.088*
C15	0.0782 (5)	0.3389 (4)	0.4027 (3)	0.0604 (10)
H15	0.0571	0.4292	0.4158	0.073*
C16	-0.0311 (4)	0.2596 (3)	0.1806 (3)	0.0390 (6)
H16	-0.0617	0.3467	0.1996	0.047*
C17	0.2484 (5)	-0.0970 (4)	0.4322 (3)	0.0552 (8)
H17A	0.1831	-0.0992	0.4930	0.066*
H17B	0.3528	-0.0202	0.4733	0.066*
C18	0.2804 (6)	-0.2441 (5)	0.3720 (4)	0.0832 (14)
H18A	0.1769	-0.3208	0.3414	0.125*

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H18B	0.3527	-0.2606	0.4315	0.125*
H18C	0.3322	-0.2449	0.3047	0.125*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ni1	0.0239 (2)	0.0277 (2)	0.0327 (2)	0.00622 (17)	0.00861 (17)	0.01208 (19)
Ni2	0.0308 (2)	0.0285 (2)	0.0283 (2)	0.00865 (18)	0.00732 (18)	0.01098 (18)
O1	0.0484 (11)	0.0311 (9)	0.0290 (9)	0.0129 (8)	0.0067 (8)	0.0113 (8)
O2	0.0517 (13)	0.0484 (12)	0.0514 (13)	0.0158 (10)	0.0160 (10)	0.0173 (10)
O3	0.0639 (14)	0.0438 (12)	0.0361 (10)	0.0201 (10)	0.0001 (10)	0.0152 (9)
O4	0.0470 (12)	0.0502 (13)	0.0537 (13)	0.0132 (10)	0.0147 (10)	0.0164 (11)
O5	0.0277 (9)	0.0310 (9)	0.0459 (11)	0.0057 (7)	0.0132 (8)	0.0149 (8)
O6	0.0374 (11)	0.0432 (12)	0.0731 (16)	-0.0024 (9)	0.0148 (11)	0.0170 (11)
C1	0.0303 (13)	0.0484 (16)	0.0388 (14)	0.0144 (12)	0.0129 (11)	0.0225 (12)
C2	0.0246 (12)	0.0412 (14)	0.0404 (14)	0.0104 (10)	0.0093 (10)	0.0238 (12)
C3	0.0300 (13)	0.0469 (17)	0.0530 (18)	0.0070 (12)	0.0110 (12)	0.0272 (15)
C4	0.0316 (15)	0.061 (2)	0.072 (2)	0.0021 (14)	0.0163 (15)	0.0362 (18)
C5	0.0380 (17)	0.079 (3)	0.069 (2)	0.0179 (17)	0.0286 (16)	0.036 (2)
C6	0.0414 (16)	0.065 (2)	0.0521 (18)	0.0205 (15)	0.0228 (14)	0.0239 (16)
C7	0.0367 (14)	0.0426 (15)	0.0386 (14)	0.0161 (12)	0.0154 (12)	0.0132 (12)
C8	0.0436 (18)	0.055 (2)	0.076 (3)	-0.0064 (16)	0.0034 (17)	0.0253 (19)
C9	0.073 (3)	0.060 (2)	0.064 (2)	-0.008 (2)	0.005 (2)	0.0134 (19)
C10	0.0472 (16)	0.0387 (15)	0.0354 (14)	0.0168 (13)	0.0131 (12)	0.0114 (12)
C11	0.0318 (13)	0.0374 (14)	0.0314 (13)	0.0086 (11)	0.0091 (10)	0.0110 (11)
C12	0.0423 (15)	0.0421 (15)	0.0341 (14)	0.0127 (12)	0.0064 (12)	0.0115 (12)
C13	0.084 (3)	0.064 (2)	0.0297 (15)	0.030 (2)	0.0049 (16)	0.0120 (15)
C14	0.114 (3)	0.064 (2)	0.0347 (17)	0.041 (2)	0.0089 (19)	0.0036 (16)
C15	0.093 (3)	0.0484 (19)	0.0391 (17)	0.0340 (19)	0.0151 (17)	0.0092 (14)
C16	0.0474 (16)	0.0345 (14)	0.0392 (15)	0.0176 (12)	0.0166 (12)	0.0139 (12)
C17	0.062 (2)	0.065 (2)	0.0424 (17)	0.0247 (17)	0.0015 (15)	0.0249 (16)
C18	0.118 (4)	0.077 (3)	0.062 (2)	0.057 (3)	0.000 (2)	0.027 (2)

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

Ni1—O5	1.837 (2)	C6—H6	0.9300
Ni1—O5 ⁱ	1.837 (2)	C7—H7	0.9300
Ni1—O4	1.852 (2)	C8—C9	1.491 (5)
Ni1—O4 ⁱ	1.852 (2)	C8—H8A	0.9700
Ni2—O1	1.843 (2)	C8—H8B	0.9700
Ni2—O1 ⁱⁱ	1.843 (2)	C9—H9A	0.9600
Ni2—O2 ⁱⁱ	1.851 (2)	C9—H9B	0.9600
Ni2—O2	1.851 (2)	C9—H9C	0.9600
O1—C11	1.309 (3)	C10—C11	1.405 (4)
O2—C16	1.282 (3)	C10—C15	1.406 (4)
O3—C12	1.365 (3)	C10—C16	1.438 (4)
O3—C17	1.429 (3)	C11—C12	1.430 (4)
O4—C7	1.294 (3)	C12—C13	1.369 (4)

O5—C2	1.319 (3)	C13—C14	1.402 (5)
O6—C3	1.367 (4)	C13—H13	0.9300
O6—C8	1.417 (4)	C14—C15	1.362 (5)
C1—C2	1.404 (4)	C14—H14	0.9300
C1—C6	1.412 (4)	C15—H15	0.9300
C1—C7	1.432 (4)	C16—H16	0.9300
C2—C3	1.426 (4)	C17—C18	1.502 (5)
C3—C4	1.380 (4)	C17—H17A	0.9700
C4—C5	1.391 (5)	C17—H17B	0.9700
C4—H4	0.9300	C18—H18A	0.9600
C5—C6	1.364 (5)	C18—H18B	0.9600
C5—H5	0.9300	C18—H18C	0.9600
O5—Ni1—O5 ⁱ	180	O6—C8—H8B	110.2
O5—Ni1—O4	94.16 (9)	C9—C8—H8B	110.2
O5 ⁱ —Ni1—O4	85.84 (9)	H8A—C8—H8B	108.5
O5—Ni1—O4 ⁱ	85.84 (9)	C8—C9—H9A	109.5
O5 ⁱ —Ni1—O4 ⁱ	94.16 (9)	C8—C9—H9B	109.5
O4—Ni1—O4 ⁱ	180	H9A—C9—H9B	109.5
O1—Ni2—O1 ⁱⁱ	180	C8—C9—H9C	109.5
O1—Ni2—O2 ⁱⁱ	86.30 (9)	H9A—C9—H9C	109.5
O1 ⁱⁱ —Ni2—O2 ⁱⁱ	93.70 (9)	H9B—C9—H9C	109.5
O1—Ni2—O2	93.70 (9)	C11—C10—C15	120.7 (3)
O1 ⁱⁱ —Ni2—O2	86.30 (9)	C11—C10—C16	120.0 (2)
O2 ⁱⁱ —Ni2—O2	180	C15—C10—C16	119.3 (3)
C11—O1—Ni2	126.59 (17)	O1—C11—C10	125.3 (2)
C16—O2—Ni2	127.6 (2)	O1—C11—C12	117.4 (2)
C12—O3—C17	118.6 (2)	C10—C11—C12	117.3 (2)
C7—O4—Ni1	127.6 (2)	O3—C12—C13	125.1 (3)
C2—O5—Ni1	127.62 (17)	O3—C12—C11	114.3 (2)
C3—O6—C8	118.6 (3)	C13—C12—C11	120.5 (3)
C2—C1—C6	120.1 (3)	C12—C13—C14	121.2 (3)
C2—C1—C7	120.5 (2)	C12—C13—H13	119.4
C6—C1—C7	119.4 (3)	C14—C13—H13	119.4
O5—C2—C1	125.0 (2)	C15—C14—C13	119.4 (3)
O5—C2—C3	117.0 (2)	C15—C14—H14	120.3
C1—C2—C3	118.0 (2)	C13—C14—H14	120.3
O6—C3—C4	125.7 (3)	C14—C15—C10	120.9 (3)
O6—C3—C2	114.0 (2)	C14—C15—H15	119.6
C4—C3—C2	120.3 (3)	C10—C15—H15	119.6
C3—C4—C5	120.8 (3)	O2—C16—C10	124.7 (3)
C3—C4—H4	119.6	O2—C16—H16	117.6
C5—C4—H4	119.6	C10—C16—H16	117.6
C6—C5—C4	120.2 (3)	O3—C17—C18	107.2 (3)
C6—C5—H5	119.9	O3—C17—H17A	110.3
C4—C5—H5	119.9	C18—C17—H17A	110.3
C5—C6—C1	120.6 (3)	O3—C17—H17B	110.3
C5—C6—H6	119.7	C18—C17—H17B	110.3

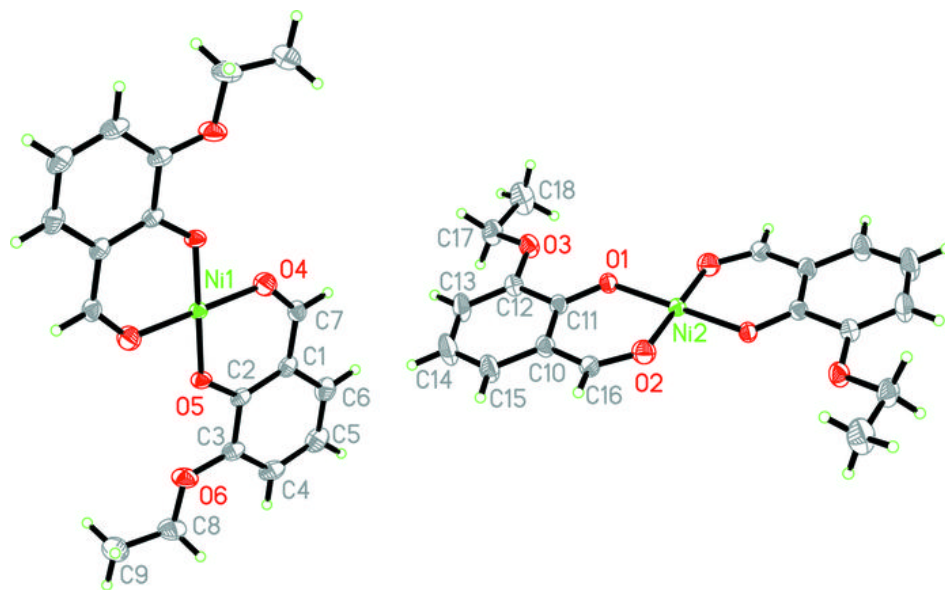
supplementary materials

C1—C6—H6	119.7	H17A—C17—H17B	108.5
O4—C7—C1	125.0 (3)	C17—C18—H18A	109.5
O4—C7—H7	117.5	C17—C18—H18B	109.5
C1—C7—H7	117.5	H18A—C18—H18B	109.5
O6—C8—C9	107.6 (3)	C17—C18—H18C	109.5
O6—C8—H8A	110.2	H18A—C18—H18C	109.5
C9—C8—H8A	110.2	H18B—C18—H18C	109.5

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x, -y, -z$.

Article retracted

Fig. 1



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