Acta Crystallographica Section E
**Structure Reports Online**
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# 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 |
|---|---|---|---|---|
| *trans-Bis{1-[3-(cyclohexylamino)propyliminomethyl]-2-naphtholato}copper(II) dichloride dihydrate* | Zhang (2004) | Journal | 10.1107/S1600536804028296 | BIPDUA |
| *Bis(4-bromo-2-formylphenolato-$\kappa^2O,O'$)copper(II)* | Sun & Gao (2005) | Author | 10.1107/S160053680500187X | FEYSUY |
| *Bis(salicylaldehydo)zinc(II)* | Xiong & Liu (2005) | Journal | 10.1107/S1600536805010913 | GAMDUU |
| *Bis(4-bromo-2-formylphenolato-$\kappa^2O,O'$)zinc(II)* | Chen (2006) | Journal | 10.1107/S1600536805040432 | SAZCUS |
| *Bis(2-formylphenolato-$\kappa^2O,O'$)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-$\kappa^2O,O'$)manganese(II)* | Wang & Fang (2006) | Journal | 10.1107/S1600536806021039 | IDOVED |
| *Tetraaqua(1,10-phenanthroline-$\kappa^2N,N'$)copper(II) naphthalene-1,5-disulfonate dihydrate* | Liu *et al.* (2006) | Author | 10.1107/S1600536806030637 | GENYOO |
| *Tetraaqua(1,10-phenanthroline-$\kappa^2N,N'$)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 *et al.* (2006) | Journal | 10.1107/S160053680604565X | HESPEB |
| *Bis(2-formylphenolato-$\kappa^2O,O'$)iron(II)* | Yang *et al.* (2007) | Author | 10.1107/S1600536807021721 | PIFCAJ |
| *2,6-Dimethoxybenzohydrazide* | Qadeer *et al.* (2007*a*) | Journal | 10.1107/S1600536807022593 | PIFHES |
| *2-(2,4-Dichlorophenylsulfanyl)acetohydrazide* | Qadeer *et al.* (2007*b*) | Journal | 10.1107/S1600536807022891 | YIFSOW |
| *{6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratoeuropium(III)zinc(II)* | Hu *et al.* (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 *et al.* (2007) | Author | 10.1107/S1600536807032540 | WIHRIP |
| *{μ-6,6′-Diethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato}-trinitratopraseodymium(III)nickel(II)* | Sui, Li *et al.* (2007) | Author | 10.1107/S1600536807032618 | UFACUA |
| *{6,6′-Dimethoxy-2,2′-[ethane-1,2-diylbis(nitrilomethylidyne)]diphenolato-1$\kappa^4O^1,O^{1'},O^6,O^{6'}$:2$\kappa^4O^1,N,N',O^{1'}$}(methanol-1κO)-μ-nitrato-1:2$\kappa^2O$:O′-dinitrato-1$\kappa^4O,O'$-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-nitrato-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-nitrato-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-nitrato-dinitratolutetium(III)zinc(II)* | Sui, Sui *et al.* (2007) | Author | 10.1107/S1600536807037737 | AFEFOH |
| *catena-Poly[[chloridonickel(II)]-di-μ-chlorido-[chloridonickel(II)]-μ-4,4′-methylenebis(3,5-dimethylpyrazole)-$\kappa^2N^2$:$N^{2'}$]* | Huang & Chen (2007) | Author | 10.1107/S1600536807039384 | VIJYOD |
| *{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}zinc(II)* | Liu *et al.* (2007*a*) | Author | 10.1107/S1600536807040640 | DIKYUS |
| *trans-Bis(ethylenediamine-$\kappa^2N,N'$)bis(nitrato-κO)zinc(II)* | Liu, Zeng & Chen (2007) | Author | 10.1107/S1600536807042390 | XIKYEW |
| *[N,N′-(o-Phenylene)bis(picolinamido)-$\kappa^4N,N',N'',N'''$]cobalt(II)* | Liu & Zeng (2007*a*) | Author | 10.1107/S1600536807044571 | XILFII |
| *[N,N′-(o-Phenylene)dipicolinamide-$\kappa^4N$]nickel(II)* | Liu & Zeng (2007*b*) | Author | 10.1107/S1600536807048386 | WINWEW |
| *{2,2′-[o-Phenylenebis(nitrilomethylidyne)]diphenolato}manganese(II)* | Liu *et al.* (2007*b*) | Author | 10.1107/S1600536807052993 | VIQPIV |
| *N-(2-Amino-3-pyridyl)urea monohydrate* | Li *et al.* (2007) | Author | 10.1107/S1600536807047526 | SIMFEA |
| *N-(2-Fluorophenyl)carbamic acid monohydrate* | Yang (2007) | Author | 10.1107/S1600536807052464 | WINMOW |
| *Aqua(dimethylglyoxime-$\kappa^2N,N'$)(3,5-dinitro-2-oxidobenzoato-$\kappa^2O^1,O^2$)-copper(II)* | Liu & Wen (2007) | Author | 10.1107/S1600536807054244 | HIQCAM |
| *μ-Acetato-tri-μ-ferrocenecarboxylatobis[(N,N-dimethylformamide)-copper(II)]* | Liu, Lin *et al.* (2007) | Journal | 10.1107/S1600536807059041 | HIQQEE |

 doi:10.1107/S1600536809054300  

**Table 1 (continued)**

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

## References


Chen, Q. (2006). *Acta Cryst.* E**62**, m56–m57.
Chen, J.-R., Sui, Y., Luo, Q.-Y. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2091–m2092.
Chen, J.-R., Sui, Y., Chen, L., Wen, J.-W. & Yin, L.-Y. (2008). *Acta Cryst.* E**64**, m562–m563.
Han, Z.-Q. (2008). *Acta Cryst.* E**64**, m592.
Harrison, W. T. A., Simpson, J. & Weil, M. (2010). *Acta Cryst.* E**66**, e1–e2.
Hu, R.-H., Sui, Y., Chen, L. & He, C.-M. (2008). *Acta Cryst.* E**64**, m8–m9.
Hu, R.-H., Sui, Y., Fang, X.-N. & Chen, H.-M. (2007). *Acta Cryst.* E**63**, m2039–m2040.
Huang, C.-F. & Chen, H.-L. (2007). *Acta Cryst.* E**63**, m2356–m2357.
Huang, Q., Sui, Y.-H. & Zhang, G.-X. (2009). *Acta Cryst.* E**65**, m1161–m1162.
Li, Y.-G. & Chen, H.-J. (2006). *Acta Cryst.* E**62**, m1038–m1039.
Li, N.-G., Tao, R.-M. & Fu, B.-F. (2007). *Acta Cryst.* E**63**, o4228.
Li, Z., Zhang, X. & Pu, X. (2008). *Acta Cryst.* E**64**, m215.
Liu, J.-T. & Fan, S.-D. (2006). *Acta Cryst.* E**62**, m2507–m2508.
Liu, J.-T., Fan, S.-D. & Li, D.-Q. (2006). *Acta Cryst.* E**62**, m2165–m2166.
Liu, D., Lin, J., Xu, Y., Huang, C. & Li, X. (2007). *Acta Cryst.* E**63**, m3094.
Liu, Y.-Q. & Wen, H.-R. (2007). *Acta Cryst.* E**63**, m2928.
Liu, Y.-Q. & Zeng, X.-R. (2007*a*). *Acta Cryst.* E**63**, m2547.
Liu, Y.-Q. & Zeng, X.-R. (2007*b*). *Acta Cryst.* E**63**, m2684.
Liu, Y.-Q., Zeng, X.-R. & Chen, W.-T. (2007). *Acta Cryst.* E**63**, m2462.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*a*). *Acta Cryst.* E**63**, m2396.
Liu, Y.-Q., Zeng, X.-R., Luo, Q.-Y. & Xu, Y.-P. (2007*b*). *Acta Cryst.* E**63**, m2854.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*a*). *Acta Cryst.* E**63**, o2892.
Qadeer, G., Rama, N. H. & Chen, W.-T. (2007*b*). *Acta Cryst.* E**63**, o2932.
Qiu, X.-Y. (2006). *Acta Cryst.* E**62**, m1190–m1191.
Sui, Y., Fang, X.-N., Hu, P. & Lin, J. (2007). *Acta Cryst.* E**63**, m2135–m2136.
Sui, Y., Fang, X.-N. & Yuan, M.-W. (2007). *Acta Cryst.* E**63**, m2275–m2276.
Sui, Y., Li, X.-F., Huang, G.-S. & Wang, G.-J. (2007). *Acta Cryst.* E**63**, m2093–m2094.
Sui, Y., Sui, Y.-H., Luo, Q.-Y. & Wang, Y.-D. (2007). *Acta Cryst.* E**63**, m2277–m2278.
Sui, Y., Xiao, Y.-A., Fang, X.-N., Zeng, X.-R. & Li, M.-H. (2006). *Acta Cryst.* E**62**, m3205–m3207.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Jiang, R.-Q. (2007). *Acta Cryst.* E**63**, m2256–m2257.
Sui, Y., Zhang, J.-H., Hu, R.-H. & Yin, L.-Y. (2007). *Acta Cryst.* E**63**, m2089–m2090.
Sun, Y.-X. & Gao, G.-Z. (2005). *Acta Cryst.* E**61**, m354–m355.
Wang, Q. & Fang, X.-N. (2006). *Acta Cryst.* E**62**, m1492–m1493.
Wang, S., Yang, T., Li, Z. & Yu, X. (2009). *Acta Cryst.* E**65**, o2198.
Xiao, Y.-A., Fu, X.-K., Sui, Y., Wu, Q. & Xiong, S.-H. (2008). *Acta Cryst.* E**64**, m806–m807.
Xiao, Y.-A., Sui, Y., Yi, X.-G., Wu, J.-H. & Zhang, L.-P. (2008). *Acta Cryst.* E**64**, m804–m805.
Xiong, Z.-Y. & Liu, L.-J. (2005). *Acta Cryst.* E**61**, m863–m864.
Yang, X.-M. (2007). *Acta Cryst.* E**63**, o4453.
Yang, Y.-M., Lu, P.-C., Zhu, T.-T. & Liu, C.-H. (2007). *Acta Cryst.* E**63**, m1613.
Zhang, P. (2004). *Acta Cryst.* E**60**, m1808–m1810.

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# Bis(2-ethoxy-6-formylphenolato-$\kappa^2O^1,O^6$)nickel(II)

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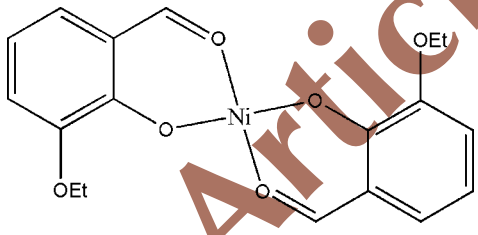
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.042; $wR$ factor = 0.116; data-to-parameter ratio = 17.3.

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 onsists 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, $P\overline{1}$
$a$ = 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) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.10 mm$^{-1}$
$T$ = 298 (2) K
0.32 × 0.32 × 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.* E**62**, m1038–m1039.
Mounts, R. D. & Fernando, Q. (1974). *Acta Cryst.* B**30**, 542–543.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Volkmer, D., Hommerich, B., Griesar, K., Haase, W. & Krebs, B. (1996). *Inorg. Chem.* **35**, 3792–3803.

# supporting information

*Acta Cryst.* (2008). E**64**, m592 [doi:10.1107/S160053680800809X]

## Bis(2-ethoxy-6-formylphenolato-$\kappa^2O^1,O^6$)nickel(II)

**Zhen-Quan Han**

### S1. 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).

### S2. 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.

### S3. 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 $U_{iso}$(H) set at 1.2$U_{eq}$(C) and 1.5$U_{eq}$(methyl C). Although no significant density was located in the solvent accessible VOIDS of 47.00 Å$^3$, these might be able to accommodate disordered water molecules.

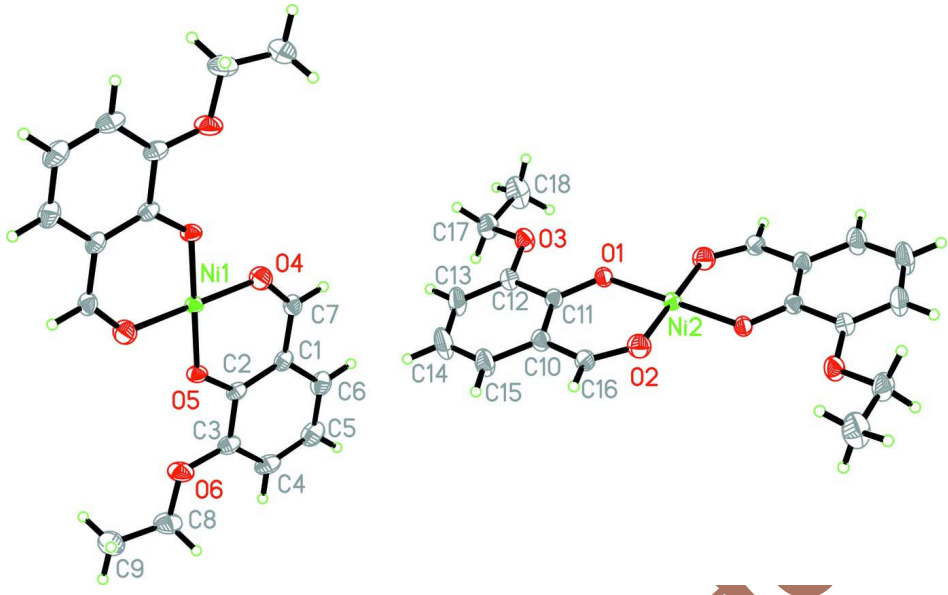



**Figure 1**

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-$\kappa^2O^1,O^6$)nickel(II)**

*Crystal data*

$[Ni(C_9H_9O_3)_2]$
$M_r = 389.03$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.448\ (2)$ Å
$b = 10.123\ (2)$ Å
$c = 11.919\ (3)$ Å
$\alpha = 111.175\ (2)°$
$\beta = 97.377\ (2)°$
$\gamma = 102.431\ (3)°$
$V = 904.1\ (4)$ Å$^3$
$Z = 2$
$F(000) = 404$
$D_x = 1.429$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2386 reflections
$\theta = 2.2–27.9°$
$\mu = 1.10$ mm$^{-1}$
$T = 298$ K
Block, red
0.32 × 0.32 × 0.30 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.719$, $T_{max} = 0.733$
5465 measured reflections
3993 independent reflections
3187 reflections with $I > 2\sigma(I)$
$R_{int} = 0.013$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.3°$
$h = -10\rightarrow8$
$k = -13\rightarrow13$
$l = -11\rightarrow15$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.116$
$S = 1.02$
3993 reflections
231 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
$w = 1/[\sigma^2(F_o^2) + (0.0596P)^2 + 0.672P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.65$ e Å$^{-3}$
$\Delta\rho_{min} = -0.66$ e Å$^{-3}$

*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 (Å²)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| 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* |
| H18B | 0.3527 | −0.2606 | 0.4315 | 0.125* |
| H18C | 0.3322 | −0.2449 | 0.3047 | 0.125* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| 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 (Å, º)*

| | | | |
|---|---|---|---|
| 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 |
| 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) $-x$, $-y$, $-z$.