Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Polymeric bis(glycolato)nickel(II)

Qing-Qing Kang, La-Sheng Long, Rong-Bin Huang* and Lan-Sun Zheng

Department of Chemistry, Xiamen University, Xiamen 361005, People's Republic of China

Correspondence e-mail: rbhuang@xmu.edu.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.021
wR factor = 0.056
Data-to-parameter ratio = 14.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

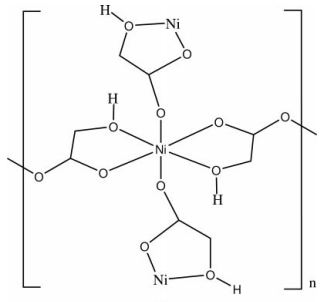
Received 4 March 2004
Accepted 11 March 2004
Online 20 March 2004

The title compound, poly[nickel(II)-bis(α-hydroxyacetato-$\kappa^3O^1,O^2:O^{1'}$)], $[Ni(C_2H_3O_3)_2]_n$, is isomorphous with the reported cobalt analogue. The Ni atom is located on a centre of inversion.

Comment

A cobalt complex of glycolate was reported by Medina *et al.* (2000). Recently, we synthesized a nickel complex of glycolate. Single-crystal X-ray diffraction analysis reveals that this complex is isomorphous with the cobalt analogue (Medina *et al.*, 2000) The Ni atom is located on a centre of inversion.

In the title compound, (I) (Fig. 1), the Ni—O distance for the carboxy O atom (Ni—O2) is shorter than that for the α-hydroxy O atom (Ni1—O1), whereas the bond length between atom Ni1 and the axially coordinated atom O3($-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$) is slightly longer than those observed for the Ni—O bonds in the chelate ring (Table 1).



(I)

Experimental

An aqueous solution of $Ni(NO_3)_2$ (1 ml, 1 mmol ml^{-1}) was added to a solution (15 ml) containing glycollic acid (0.07 g, 1 mmol) in a mixed solvent of water and ethanol in the volume ratio 1:1. The pH value of the solution was adjusted to ~5 with NaOH solution. The resulting green solution was sealed into a stainless steel autoclave. The autoclave was heated slowly to 453 K over a period of 8 h and then cooled to 393 K at a rate of 1.5 K h^{-1}. The temperature was kept at 393 K for 75 h and then allowed to drop to 303 K over a period of 8 h. Green crystals of the title compound, suitable for X-ray diffraction, were obtained.

Crystal data

$[Ni(C_2H_3O_3)_2]$
M_r = 208.80
Monoclinic, $P2_1/n$
a = 5.1304 (7) Å
b = 7.6367 (11) Å
c = 8.6076 (12) Å
β = 105.443 (2)°
V = 325.06 (8) Å^3
Z = 2
D_x = 2.133 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1462 reflections
θ = 3.6–27.9°
μ = 2.96 mm^{-1}
T = 298 (2) K
Prism, green
0.38 × 0.20 × 0.12 mm

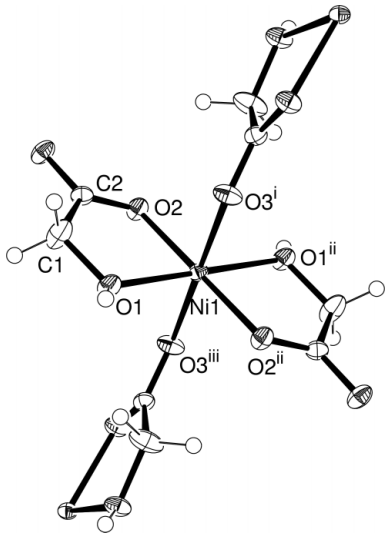


Figure 1
The coordination of the Ni^{II} ion in the title compound. Displacement ellipsoids are shown at the 50% probability level [symmetry codes: (i) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$; (ii) $1-x, 2-y, 2-z$; (iii) $\frac{1}{2}+x, \frac{3}{2}-y, \frac{1}{2}+z$].

Data collection

Bruker SMART APEX 2000 diffractometer	736 independent reflections
φ and ω scans	702 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)	$R_{int} = 0.015$
$T_{min} = 0.399$, $T_{max} = 0.718$	$\theta_{max} = 28.1°$
1829 measured reflections	$h = -5 \rightarrow 6$
	$k = -7 \rightarrow 9$
	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0283P)^2 + 0.1923P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.021$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.056$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
$S = 1.11$	$\Delta\rho_{min} = -0.36$ e Å^{-3}
736 reflections	
52 parameters	
H-atom parameters constrained	

Table 1
Selected geometric parameters (Å, °).

Ni1—O2	2.0095 (12)	Ni1—O3^{i}	2.0899 (12)
Ni1—O1	2.0374 (12)		
O2—Ni1—O1^{ii}	99.99 (5)	O1—Ni1—O3^{i}	88.19 (5)
O2—Ni1—O1	80.01 (5)		

Symmetry codes: (i) $\frac{1}{2}-x, \frac{1}{2}+y, \frac{3}{2}-z$; (ii) $1-x, 2-y, 2-z$.

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1*C*···O3^{iv}	0.82	1.84	2.6568 (17)	177

Symmetry code: (iv) $x-\frac{1}{2}, \frac{3}{2}-y, \frac{1}{2}+z$.

H atoms were treated as riding, with C—H = 0.97 Å, O—H = 0.82 Å, and $U_{iso}(H) = 1.2U_{eq}(C)$ and $1.5U_{eq}(O)$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

The authors thank the Fujian Institute of Research on the Structure of Materials (grant No. 020047).

References

Bruker (2001). *SAINT* and *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Johnson, C. K. (1976). *ORTEP*II. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Medina, G., Gasque, L. & Bernès, S. (2000). *Acta Cryst.* C**56**, 637–638.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.