Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

catena-Poly[[[tetraaquanickel(II)]-μ-glycine-κ^2O:O'] dinitrate]

Michel Fleck[a]* and Ladislav Bohatý[b]

[a]Universität Wien – Geozentrum, Institut für Mineralogie und Kristallographie, Althanstraße 14, A-1090 Wien, Austria, and [b]Universität zu Köln, Institut für Kristallographie, Zülpicher Strasse 49b, D 50674 Köln, Germany

Correspondence e-mail:
michel.fleck@univie.ac.at

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.030
wR factor = 0.082
Data-to-parameter ratio = 20.7

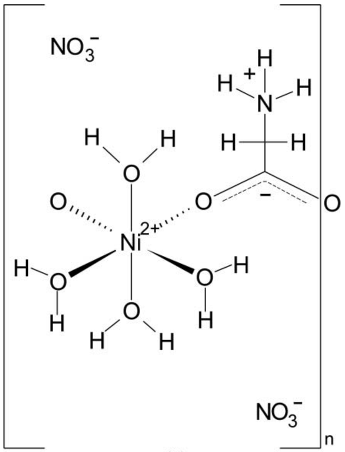
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The title compound, $\{[Ni(C_2H_5NO_2)(H_2O)_4](NO_3)_2\}_n$, contains *cis*-$NiO_2(H_2O)_4$ octahedra linked by the glycine molecules into helical chains. Its structural relationship to other glycine metal nitrates is discussed.

Received 11 August 2005
Accepted 24 August 2005
Online 31 August 2005

Comment

The title compound, (I), is isostructural with glycine magnesium nitrate tetrahydrate (Fleck & Bohatý, 2005) and glycine cobalt nitrate tetrahydrate (Clegg *et al.*, 1987). A detailed description of the structure can be found in the previous paper (Fleck & Bohatý, 2005). The interatomic distances (Table 1) and angles in (I) are similar to those in the Mg compound [Ni—O 2.031 (1)–2.080 (1) Å, C—O1 and C—O2 1.249 (2) and 1.254 (2) Å, respectively, and O2—C1—C2—N3 179.54 (1)°].



(I)

We will now survey the crystallochemical situation of all structurally known glycine metal nitrate compounds with respect to the shape and connectivity of their coordination polyhedra. Since the various metal cations are different in charge and ionic radii, most structures are unique. There is only one group of isostructural compounds, namely the glycine M^{II} nitrate tetrahydrates, with M^{II} = Mg (Fleck & Bohatý, 2005), Co (Clegg *et al.*, 1987) and the title compound. In glycine lithium nitrate (Baran *et al.*, 2003), pairs of $[LiO_4]$ tetrahedra form edge-sharing dimers, which are in turn connected by glycine molecules into infinite chains along [100]. The glycine molecules act as bridging ligands between the chains (Fig. 2*a*). In glycine sodium nitrate (Krishnakumar *et al.*, 2001), there are layers of $[NaO_8]$ polyhedra. The polyhedra resemble ditrigonal bipyramids, and each is connected to three adjacent polyhedra by common corners. The gaps

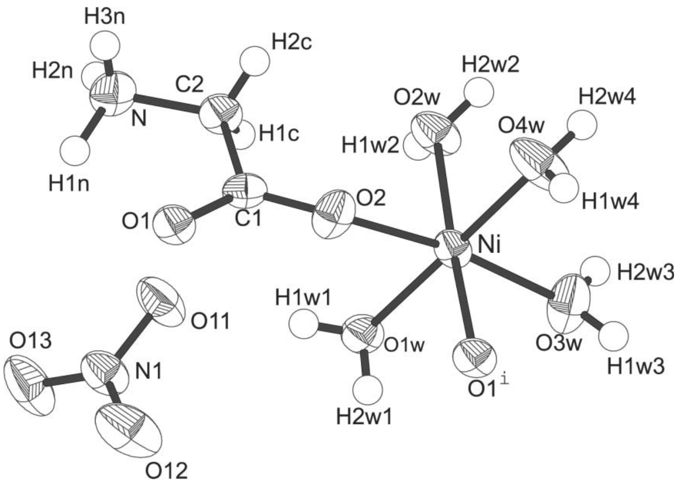


Figure 1

The connectivity in (I), shown with displacement ellipsoids at the 50% probability level. [Symmetry code: (i) $-x + \frac{1}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$.]

between three neighbouring bipyramids are filled by the nitrate groups. The apices of these bipyramids are O atoms from the carboxylate groups of the glycine molecules, connecting two layers (Fig. 2*c*).

The structure of glycine silver nitrate (Mohana Rao & Viswamitra, 1972) is characterized by groups of two glycine molecules coordinating two Ag^I cations, the glycine molecules acting as bridging ligands (Fig. 2*b*). The structure of copper glycinate nitrate monohydrate (Davies *et al.*, 1992) is unique in several ways. It is the only structure where the glycine N atom is part of the coordination sphere of the cation. This is possible since the amino group is not protonated, and thus the lone pair electrons of the N atom can interact with the Cu^{II} cation. Consequently, the glycine molecules act as N,O-bidentate ligands and the other O atom of the carboxylate group bonds to a neighbouring cation. The Cu coordination polyhedron can be described as a typical [4+1] tetragonal pyramid. Both ligands of the bidentate glycine molecules are part of the square, and the apex of the pyramid is atom O1 of another glycine molecule. Overall, two pyramids and two glycine molecules are connected to form a dimer (Fig. 2*d*).

In glycine calcium nitrate dihydrate (Natarajan *et al.*, 1984), the Ca^{II} cations are irregularly eightfold coordinated. Each $[CaO_8]$ polyhedron shares common edges with two adjacent polyhedra, thus building an infinite chain parallel to [100], enclosing a twofold screw axis (Fig. 3*a*). Since the centres of the polyhedra are located off the axis, the chain has a slight zigzag appearance. The O atoms of the common edges are part of the carboxylate groups of the glycine molecules that are located in each apex of the zigzag chain and which face away from the chain axis. Two other O atoms are from water molecules, and two O atoms belong to a nitrate group that shares an edge with the $[CaO_8]$ polyhedron. The other nitrate group is isolated from the chains and connected only *via* hydrogen bonds. As might be expected for large cations, the carboxylate groups act as bidentate ligands. This compound is the only member in the group of structurally known glycine metal nitrate compounds where the carboxylate group acts as a bidentate ligand only. However, there are other compounds of glycine with inorganic salts for which this is also the case. In particular, bis(glycine) barium dichloride and bis(glycine) strontium dichloride (Narayanan & Venkataraman, 1975) show this feature. In tris(glycine) calcium chloride (Ravikumar *et al.*, 1986), there are different glycine molecules, acting as either bridging or bidentate ligands of Ca^{II} cations. These cations are seven-coordinated and the coordination polyhedra are shaped like distorted pentagonal bipyramids, each including one Cl^- anion. Two such bipyramids share one common edge, and these dimers are connected by the glycine molecules to infinite layers parallel to (010) (Fig. 3*b*).

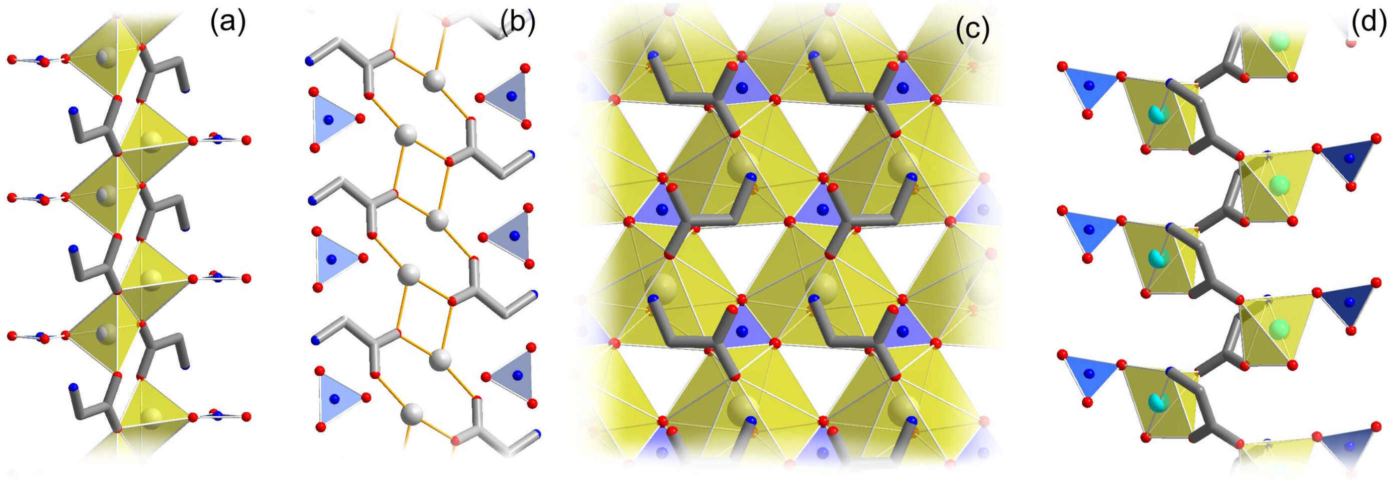


Figure 2

A comparison of building units in glycine metal nitrates. (*a*) View of a chain of double LiO_4 tetrahedra connected by glycine molecules in glycine $Li(NO_3)$ (Baran *et al.*, 2003). (*b*) View of the structure of glycine $Ag(NO_3)$ (Mohana Rao & Viswamitra, 1972). (*c*) View of a layer of corner-sharing NaO_8 bipyramids in glycine $Na(NO_3)$ (Krishnakumar *et al.*, 2001). (*d*) View of the structure of Cu glycinate $(NO_3)\cdot H_2O$ (Davies *et al.*, 1992). Note the chain of CuO_4N pyramids connected by glycine molecules that are both bidentate and bridging. The $M-O$ polyhedra are yellow, the NO_3 groups are blue, the glycine molecules are represented by a stick model, and H atoms have been omitted for clarity.

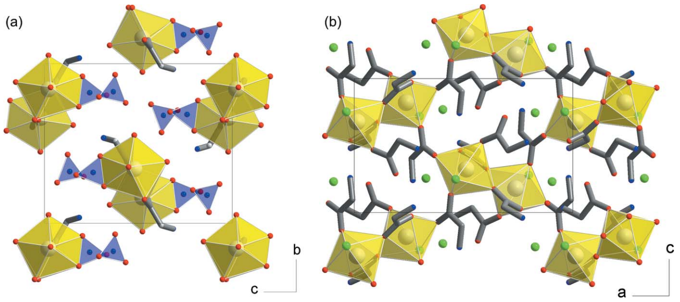


Figure 3
(*a*) A packing diagram for glycine calcium nitrate dihydrate (Natarajan *et al.*, 1984). (*b*) Comparison with tris(glycine) calcium chloride (Ravikumar *et al.*, 1986). (*a*) is viewed along the chains parallel to [100], (*b*) on to a layer parallel to (010). Note the role of the glycine molecules: in (*a*), there is only one glycine as a bidentate ligand, while in (*b*) there are six, as unidentate, bidentate and bridging ligands.

Experimental

A stoichiometric mixture of glycine and nickel(II) nitrate was dissolved in water. The resulting solution was slowly evaporated at a temperature of approximately 295 K over a period of several weeks, to yield green crystals of (I) up to 2 mm in size.

Crystal data

$[Ni(C_2H_5NO_2)(H_2O)_4](NO_3)_2$
$M_r = 329.86$
Monoclinic, $P2_1/n$
$a = 9.201\ (1)$ Å
$b = 6.773\ (1)$ Å
$c = 18.966\ (2)$ Å
$\beta = 96.775\ (1)°$
$V = 1173.7\ (2)$ Å^3
$Z = 4$
$D_x = 1.867$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4780 reflections
$\theta = 4.1$–$33.1°$
$\mu = 1.72$ mm^{-1}
$T = 293\ (2)$ K
Irregular fragment, green
0.08 × 0.05 × 0.04 mm

Data collection

Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*DENZO-SMN*; Otwinowski & Minor, 1997)
$T_{min} = 0.875$, $T_{max} = 0.934$
7769 measured reflections
4462 independent reflections
3240 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 35.0°$
$h = -14 \rightarrow 14$
$k = -10 \rightarrow 8$
$l = -30 \rightarrow 30$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.030$
$wR(F^2) = 0.082$
$S = 1.01$
4462 reflections
216 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.04P)^2 + 0.25P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.47$ e Å^{-3}
$\Delta\rho_{min} = -0.35$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.0081 (10)

Table 1
Selected geometric parameters (Å).

Ni1—O2*W*	2.0316 (12)	Ni1—O2^i	2.0518 (11)
Ni1—O4*W*	2.0339 (13)	Ni1—O3*W*	2.0584 (14)
Ni1—O1	2.0491 (11)	Ni1—O1*W*	2.0803 (11)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H1N···O23^{ii}	0.96 (3)	2.03 (3)	2.948 (2)	160 (2)
N—H2N···O11	0.90 (3)	2.03 (3)	2.933 (2)	176 (2)
N—H3N···O22^{iii}	0.82 (3)	2.34 (3)	3.024 (2)	142 (3)
O1*W*—H1*W*1···O11^{iv}	0.86 (3)	1.95 (3)	2.7876 (18)	163 (2)
O1*W*—H2*W*1···O2	0.78 (3)	1.97 (3)	2.7037 (15)	156 (2)
O2*W*—H1*W*2···O22^{v}	0.70 (3)	2.12 (3)	2.793 (2)	163 (3)
O2*W*—H2*W*2···O13^{vi}	0.88 (3)	1.91 (3)	2.7851 (18)	171 (2)
O3*W*—H1*W*3···O12^{vii}	0.77 (3)	2.07 (3)	2.812 (2)	162 (2)
O3*W*—H2*W*3···O21	0.77 (2)	2.04 (3)	2.788 (2)	162 (2)
O4*W*—H1*W*4···O23^{ii}	0.71 (2)	2.13 (2)	2.836 (2)	174 (3)
O4*W*—H2*W*4···O12^{vi}	0.88 (3)	1.88 (3)	2.754 (2)	173 (2)

Symmetry codes: (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (v) $-x+1, -y, -z$; (vi) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (vii) $-x+1, -y, -z+1$.

Table 3
Overview of the stoichiometry, symmetries and unit-cell parameters of glycine metal nitrate compounds (Å, °).

Compound	*a*	*b*	*c*	α	β	γ	Space group	Ref.
$C_2H_5N_2{\cdot}Li(NO_3)$	5.59	5.90	8.66	92.1	92.79	97.1	$P\bar{1}$	(*a*)
$C_2H_5N_2{\cdot}Na(NO_3)$	14.32	5.26	9.11	90	119.07	90	*Cc*	(*a*), (*b*)
$C_2H_5N_2{\cdot}Ag(NO_3)$	5.45	19.49	5.54	90	100.20	90	$P2_1$	(*c*)
$C_2H_5N_2{\cdot}Ca(NO_3)_2{\cdot}2H_2O$	6.87	11.27	13.25	90	90	90	$P2_12_12_1$	(*d*)
$C_2H_5N_2{\cdot}Mg(NO_3)_2{\cdot}4H_2O$	9.23	6.78	19.05	90	96.57	90	$P2_1/n$	(*e*)
$C_2H_5N_2{\cdot}Ni(NO_3)_2{\cdot}4H_2O$	9.20	6.77	18.97	90	96.77	90	$P2_1/n$	(*f*)
$C_2H_5N_2{\cdot}Co(NO_3)_2{\cdot}4H_2O$	9.24	6.72	19.04	90	96.51	90	$P2_1/n$	(*g*)
$C_2H_4N_2{\cdot}Cu(NO_3){\cdot}H_2O$	9.28	5.18	13.97	90	103.29	90	$P2_1/n$	(*h*)

References: (*a*) Baran *et al.* (2003); (*b*) Krishnakumar *et al.* (2001); (*c*) Mohana Rao & Viswamitra (1972); (*d*) Natarajan *et al.* (1984); (*e*) Fleck & Bohaty (2005); (*f*) this work; (*g*) Clegg *et al.* (1987); (*h*) Davies *et al.* (1992).

All H atoms were located in difference maps and freely refined.

Data collection: *COLLECT* (Nonius, 2003); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff *et al.*, 1996) and *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

The authors thank the International Centre for Diffraction Data for financial assistance for this work (grant No. 90-03 ET).

References

Baran, J., Drozd, M., Pietraszko, A., Trzebiatowska, M. & Ratajczak, H. (2003). *Polish J. Chem.* **77**, 1561–1577.
Bergerhoff, G., Berndt, M. & Brandenburg, K. (1996). *J. Res. Natl Inst. Stand. Technol.* **101**, 221–225.
Clegg, W., Lacy, O. M. & Straughan, B. P. (1987). *Acta Cryst.* C**43**, 794–797.
Davies, H. O., Gillard, R. D., Hursthouse, M. B., Mazid, M. A. & Williams, P. A. (1992). *J. Chem. Soc. Chem. Commun.* pp. 226–230.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Fleck, M. & Bohatý, L. (2005). *Acta Cryst.* E**61**, m1887–m1889.
Krishnakumar, R. V., Subha Nandhini, M., Natarajan, S., Sivakumar, K. & Varghese, B. (2001). *Acta Cryst.* C**57**, 1149–1150.
Mohana Rao, J. K. & Viswamitra, M. A. (1972). *Acta Cryst.* B**28**, 1484–1496.
Narayanan P. & Venkataraman, S. (1975). *Z. Kristallogr.* **142**, 52–81.
Natarajan, S., Ravikumar, K. & Rajan, S. S. (1984). *Z. Kristallogr.* **168**, 75–79.

Nonius (2003). *COLLECT*. Nonius BV, Delft, The Netherlands.

Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.

Ravikumar, K., Rajan, S. S., Natarajan, S., Ponnuswamy, M. N. & Trotter, J. (1986). *Z. Kristallogr.* **175**, 217–225.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.