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Poly[[[diaquacobalt(II)]-di-μ-glycine] dichloride]

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.022
wR factor = 0.058
Data-to-parameter ratio = 13.9

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

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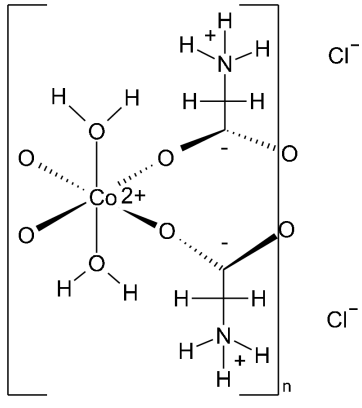
The crystal structure of the title compound, $\{[Co(C_2H_5NO_2)_2(H_2O)_2]Cl_2\}_n$, is presented and compared with other compounds of glycine and M^{II} chlorides. It contains CoO_6 octahedra connected by glycine molecules into layers. The Co atoms lie on centres of inversion. Chloride ions are located between the layers. It is the first known example of a glycine–M^{II} chloride with a glycine–metal ratio of 2:1.

Comment

In the course of our studies of new compounds of glycine and inorganic materials (Fleck & Bohatý, 2004) we have investigated the system glycine–cobalt chloride–water. Besides the already known structure of a dihydrated 1:1 glycine–cobalt complex, $(C_2H_5NO_2)CoCl_2\cdot 2H_2O$ (Clegg *et al.*, 1987), we have found a new member of this system, with a 2:1 glycine–cobalt ratio, (I). The main structural feature of this compound is the coordination polyhedron of the Co atom on a centre of inversion. It can be described as a slightly distorted octahedron, the ligands being six O atoms. Four of these O atoms belong to glycine molecules, two are from water molecules. The octahedra are connected to each other by four glycine molecules, forming layers parallel to (100). The glycine molecules are more or less perpendicular to the layers, the amino groups facing away from the layers. Chloride ions are located in the interstices between the glycine molecules, thus connecting adjacent layers by hydrogen bonds from the amino groups as well as the water molecules.



(I)

In contrast to this structure the atomic arrangement in the earlier 1:! complex (Clegg *et al.*, 1987) is completely different. The Co atom is also six-coordinate, but two ligands are Cl atoms and four are O atoms. Two of these belong to water molecules, the other two are part of glycine molecules. Because of the two long Co—Cl bonds 2.3988 (7) and

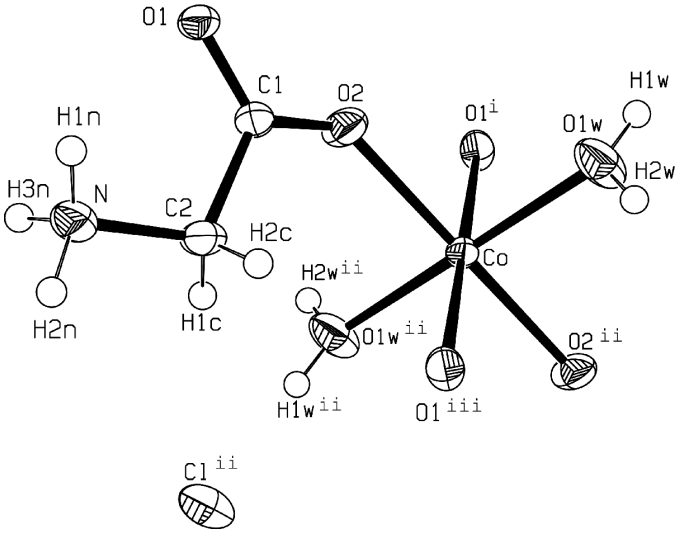


Figure 1
The connectivity in (I), shown with displacement ellipsoids at the 50% probability level (*ORTEP*3; Farrugia, 1997). The symmetry codes are the same as those in Table 1.

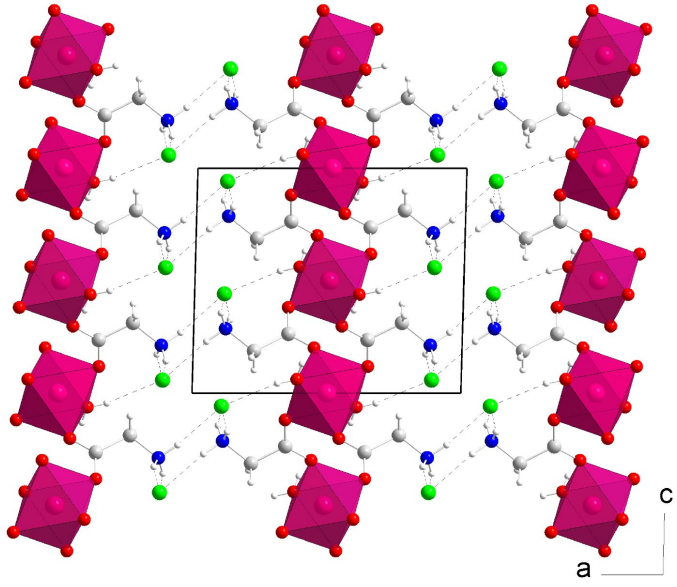


Figure 2
Packing diagram (*DIAMOND*; Bergerhoff *et al.*, 1997) of (I), viewed along [010]. The layers are oriented vertically.

2.4972 (7) Å], the coordination polyhedron can be described as a rather distorted octahedron. Each of these octahedra is connected to two other octahedra by glycine molecules, thus forming a zigzag chain along [101]. The chains are connected to each other by hydrogen bonds, from the H atoms of the amino group to chloride ligands and water molecules, and from the water molecules to Cl and to O atoms of the acid groups.

Experimental

Crystals of the title compound were grown from aqueous solutions of glycine and cobalt chloride hexahydrate in the following ratio: 1.98 g cobalt chloride hexahydrate and 1.42 g glycine. The solution was slowly evaporated at a temperature of approximately 295 K over a period of several weeks. The synthesis yielded crystals up to several mm in size.

Crystal data

$[Co(C_2H_5NO_2)_2(H_2O)_2]\cdot Cl_2$
$M_r = 316.00$
Monoclinic, $P2_1/c$
$a = 10.568$ (2) Å
$b = 5.988$ (1) Å
$c = 8.844$ (2) Å
$\beta = 91.55$ (3)°
$V = 559.45$ (19) Å^3
$Z = 2$
$D_x = 1.876$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1496 reflections
$\theta = 2.0$–28.3°
$\mu = 2.02$ mm^{-1}
$T = 293$ (2) K
Fragment, pink
0.30 × 0.30 × 0.10 mm

Data collection

Nonius KappaCCD diffractometer
φ and ω scans
Absorption correction: multi-scan (*SCALEPACK*; Otwinowski & Minor, 1997)
$T_{min} = 0.582$, $T_{max} = 0.823$
2525 measured reflections
1376 independent reflections
1274 reflections with $I > 2\sigma(I)$
$R_{int} = 0.012$
$\theta_{max} = 28.3°$
$h = -14 \rightarrow 14$
$k = -7 \rightarrow 7$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.022$
$wR(F^2) = 0.058$
$S = 1.08$
1376 reflections
99 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0275P)^2 + 0.3111P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.57$ e Å^{-3}
$\Delta\rho_{min} = -0.50$ e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.033 (3)

Table 1
Selected bond lengths (Å).

Co—O1*W*	2.0673 (14)	Co—O1^{iii}	2.0924 (11)
Co—O1*W*^{i}	2.0673 (14)	Co—O2^{i}	2.1031 (11)
Co—O1^{ii}	2.0924 (11)	Co—O2	2.1031 (11)

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

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N—H1N···Cl^{iv}	0.90 (3)	2.41 (3)	3.2905 (17)	163 (2)
N—H2N···Cl	0.91 (3)	2.30 (3)	3.2002 (17)	169 (2)
N—H1N···Cl^{iv}	0.90 (3)	2.41 (3)	3.2905 (17)	163 (2)
O1*W*—H1*W*···Cl^{v}	0.79 (3)	2.38 (3)	3.1457 (17)	167 (3)
O1*W*—H2*W*···O2^{ii}	0.70 (3)	2.16 (3)	2.768 (2)	146 (3)

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

Data collection: *COLLECT* (Nonius, 2003); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff *et al.*, 1997) and *ORTEP*3 (Farrugia, 1997); software used to prepare material for publication: *SHELXL*97.

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References

Bergerhoff, G., Berndt, M. & Brandenburg, K. (1997). *J. Res. Natl. Inst. Stand. Technol.*, **101**, 221–225.
Clegg, W., Lacy, O. M. & Straughan, B. P. (1987). *Acta Cryst.* C**43**, 794–797.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Fleck, M. & Bohatý, L. (2004). *Acta Cryst.* C**60**, m291–m295.
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 and R. M. Sweet, pp. 307–326. New York: Academic Press.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.