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Dichloridodiglycinezinc dihydrate

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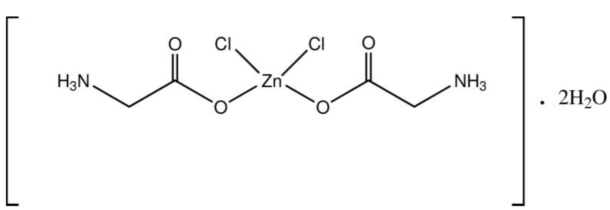
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.002 Å; R factor = 0.013; wR factor = 0.034; data-to-parameter ratio = 11.2.

The title compound, $[ZnCl_2(C_2H_5NO_2)_2]\cdot 2H_2O$, crystallizes with one half-molecule in the asymmetric unit and a twofold rotation axis passing through the Zn atom. The glycine molecules are zwitterionic. The eight water molecules present in the unit cell mediate the formation of a three-dimensional hydrogen-bonded network in the crystal structure.

Related literature

For related crystal structures, see: Hariharan *et al.* (1989).



Experimental

Crystal data

$[ZnCl_2(C_2H_5NO_2)_2]\cdot 2H_2O$
M_r = 322.46
Monoclinic, $C2/c$
a = 14.4167 (11) Å
b = 6.9068 (4) Å
c = 12.9531 (7) Å
β = 117.940 (4)°
V = 1139.44 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.64 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (Blessing, 1995)
T_{min} = 0.578, T_{max} = 0.782 (expected range = 0.436–0.590)
9969 measured reflections
1008 independent reflections
1004 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.013
$wR(F^2)$ = 0.034
S = 1.12
1008 reflections
90 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3A···O1^{i}	0.84 (2)	2.04 (2)	2.8812 (15)	175 (2)
O3—H3B···O1^{ii}	0.76 (2)	2.16 (2)	2.9163 (16)	172 (2)
N1—H1C···O3^{iii}	0.90 (2)	1.97 (2)	2.8714 (18)	177.4 (17)
N1—H1A···O1^{i}	0.87 (2)	2.40 (2)	3.1707 (18)	147.4 (17)
N1—H1B···O3^{iv}	0.80 (2)	2.09 (2)	2.8891 (18)	170.5 (18)

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

Data collection: *APEX2* (Bruker Nonius, 2004); cell refinement: *APEX2* and *SAINT-Plus* (Bruker Nonius, 2004); data reduction: *SAINT-Plus* and *XPREP* (Bruker Nonius, 2004); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97* and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RK2031).

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supplementary materials

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Comment

Some aminoacids and their complexes are of considerable chemical, optical and biological interest. As part of our ongoing research for finding new nonlinear optics (NLO) materials. We are attempting grow fairly big crystals of aminoacid metal complexes. Crystal structure of dichloro-*bis*(glycine-O)-zinc glycine (Hariharan *et al.*, 1989), is an NLO material. During our attempt to synthesize this compound, we found that, a new complex, namely, dichloro-*bis*(glycine)-zinc dihydrate (I), is also formed along with. As the compound is new, it was decided to elucidate its crystal structure. The molecule crystallizes in monoclinic system with space group *C*2/*c* with half the molecule in the asymmetric unit. The two–fold axis passing through the Zn atom bisects the molecule. In the crystal structure, zinc atom is tetrahedrally coordinated with two molecules of chlorine and one oxygen each of the carboxyl groups of the glycine. Both glycine molecules are zwitterionic. There are two water molecules in the assymetric unit. The structure packing formes a three dimensional network of hydrogen bonds. The water molecules mediate N—H—O hydrogen bonded link between different units of (I). There are no direct hydrogen bonded link betwen glycine zinc chloride molecules.

Experimental

A supersaturated solution of glycine zinc chloride complex was prepared by dissolving equimolar amounts of glycine and $ZnCl_2$ and stirring continuously using magnetic a stirrer for 12 h. The prepared solution was filtered and kept at room temperature. Crystals were formed in three days. Inspection showed that the crystals were of of two different morphologies. X-ray indexing of these identified them to be belonging to two different complexes *viz*; dichloro-*bis*(glycine-O)-zinc glycine (Hariharan *et al.*, 1989) and the title compound (I). Crystals of (I) had diamond shaped morphology while that of the other was irregular polyhedra. The melting point of the material was measured by capillary method using Silicon oil melting point apparatus. The compound melts at 376 K. Thermogravimetric analysis was done using the instrument NETZSCH STA 409 C/CD, which showed the first sharp weight loss starting close to 400 K. This weightloss is assigned to loss of water showing that water is present in the complex after melting.

Refinement

All the hydrogen atoms were located in difference Fourier map. Water H atoms were isotropically refined. The CH_2 hydrogen atoms were geometrically fixed (0.97 Å) and given riding model refinement with U_{iso} equal to 1.2 U_{eq}C. Program shell used for structure solution, refinement, analysis and graphics - *WinGX* (Farrugia, 1999).

Figures

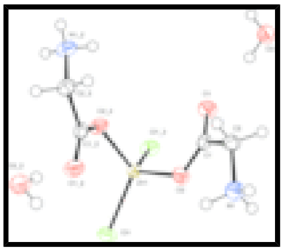

Fig. 1. The molecule structure of the title compound with atom labels and 50% probability displacement ellipsoids for non-H atoms. H atoms presented as spheres with arbitrary radius. Symmetry code _2: $2 - x$, y, $0.5 - z$.

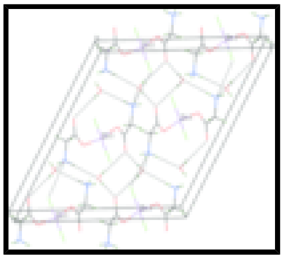

Fig. 2. Packing of molecules in the unit cell. Hydrogen bonds are shown with dotted lines.

Dichloridodiglycinezinc dihydrate

Crystal data

$[ZnCl_2(C_2H_5NO_2)_2]\cdot 2H_2O$	$F_{000} = 656$
$M_r = 322.46$	$D_x = 1.880$ Mg m^{-3}
Monoclinic, $C2/c$	Melting point: 376 K
Hall symbol: -C 2yc	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 14.4167$ (11) Å	Cell parameters from 7181 reflections
$b = 6.9068$ (4) Å	$\theta = 2.8$–25.0°
$c = 12.9531$ (7) Å	$\mu = 2.64$ mm^{-1}
$\beta = 117.940$ (4)°	$T = 293$ (2) K
$V = 1139.44$ (13) Å^3	Prism, colourless
$Z = 4$	$0.30 \times 0.20 \times 0.20$ mm

Data collection

Bruker Kappa APEXII CCD diffractometer	1008 independent reflections
Radiation source: fine–focus sealed tube	1004 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.031$
$T = 293(2)$ K	$\theta_{max} = 25.0$°
ω and φ scans	$\theta_{min} = 3.2$°
Absorption correction: multi-scan (Blessing, 1995)	$h = -17 \rightarrow 17$
$T_{min} = 0.578$, $T_{max} = 0.782$	$k = -8 \rightarrow 8$
9969 measured reflections	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.013$	$w = 1/[\sigma^2(F_o^2) + (0.015P)^2 + 0.7575P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.034$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.12$	$\Delta\rho_{max} = 0.22$ e Å^{-3}
1008 reflections	$\Delta\rho_{min} = -0.18$ e Å^{-3}
90 parameters	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0604 (12)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\sigma(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	1.0000	0.28907 (3)	0.2500	0.01935 (11)
Cl1	0.86678 (2)	0.09616 (5)	0.13652 (3)	0.03154 (12)
O1	1.10441 (7)	0.59018 (14)	0.45232 (9)	0.0307 (2)
O2	0.94677 (7)	0.47738 (14)	0.32473 (8)	0.0277 (2)
C1	1.00740 (10)	0.60066 (18)	0.39672 (11)	0.0208 (3)
C2	0.95567 (10)	0.77847 (18)	0.41474 (12)	0.0236 (3)
H2A	0.9870	0.8065	0.4977	0.028*
H2B	0.9693	0.8880	0.3769	0.028*
N1	0.84174 (10)	0.7565 (2)	0.36831 (12)	0.0292 (3)
H1C	0.8099 (15)	0.723 (3)	0.2924 (19)	0.041 (5)*
H1A	0.8292 (15)	0.671 (3)	0.4096 (18)	0.046 (5)*
H1B	0.8166 (15)	0.857 (3)	0.3742 (16)	0.042 (5)*
O3	0.76138 (9)	0.13810 (16)	0.37226 (9)	0.0302 (2)
H3A	0.8038 (19)	0.214 (3)	0.423 (2)	0.055 (6)*
H3B	0.7180 (17)	0.118 (3)	0.3885 (17)	0.049 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.02036 (14)	0.01750 (15)	0.02109 (14)	0.000	0.01046 (10)	0.000
Cl1	0.02259 (18)	0.0314 (2)	0.0375 (2)	−0.00571 (13)	0.01148 (15)	−0.01057 (14)
O1	0.0224 (5)	0.0349 (5)	0.0334 (5)	0.0025 (4)	0.0118 (4)	−0.0037 (4)
O2	0.0265 (5)	0.0256 (5)	0.0321 (5)	−0.0006 (4)	0.0148 (4)	−0.0092 (4)
C1	0.0249 (7)	0.0215 (6)	0.0202 (6)	−0.0001 (5)	0.0139 (5)	0.0010 (5)
C2	0.0240 (7)	0.0199 (6)	0.0285 (7)	−0.0018 (5)	0.0137 (5)	−0.0038 (5)
N1	0.0244 (6)	0.0281 (6)	0.0365 (7)	0.0018 (5)	0.0155 (6)	−0.0072 (6)
O3	0.0261 (5)	0.0342 (6)	0.0294 (5)	0.0022 (5)	0.0124 (5)	−0.0033 (4)

Geometric parameters (Å, °)

Zn1—Cl1	2.2314 (4)	C1—O1	1.2394 (16)
Zn1—Cl1^{i}	2.2314 (4)	C1—O2	1.2623 (16)
Zn1—O2	1.9783 (9)	N1—H1C	0.90 (2)
Zn1—O2^{i}	1.9783 (9)	N1—H1A	0.87 (2)
C2—N1	1.4684 (18)	N1—H1B	0.80 (2)
C2—C1	1.5107 (17)	O3—H3A	0.84 (2)
C2—H2A	0.9700	O3—H3B	0.76 (2)
C2—H2B	0.9700		
N1—C2—C1	113.07 (11)	C2—N1—H1B	109.9 (13)
N1—C2—H2A	109.0	H1C—N1—H1B	107.7 (17)
C1—C2—H2A	109.0	H1A—N1—H1B	107.2 (18)
N1—C2—H2B	109.0	C1—O2—Zn1	120.75 (8)
C1—C2—H2B	109.0	H3A—O3—H3B	107 (2)
H2A—C2—H2B	107.8	O2—Zn1—O2^{i}	97.79 (6)
O1—C1—O2	126.28 (12)	O2—Zn1—Cl1	107.64 (3)
O1—C1—C2	117.56 (11)	O2^{i}—Zn1—Cl1	118.79 (3)
O2—C1—C2	116.16 (11)	O2—Zn1—Cl1^{i}	118.81 (3)
C2—N1—H1C	112.0 (12)	O2^{i}—Zn1—Cl1^{i}	107.69 (3)
C2—N1—H1A	109.4 (13)	Cl1—Zn1—Cl1^{i}	106.67 (2)
H1C—N1—H1A	110.6 (17)		
N1—C2—C1—O1	−166.07 (12)	C1—O2—Zn1—O2^{i}	−58.56 (9)
N1—C2—C1—O2	14.67 (17)	C1—O2—Zn1—Cl1	177.83 (9)
O1—C1—O2—Zn1	−20.74 (18)	C1—O2—Zn1—Cl1^{i}	56.60 (10)
C2—C1—O2—Zn1	158.44 (8)		

Symmetry codes: (i) $-x+2, y, -z+1/2$.

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O3—H3A···O1^{ii}	0.84 (2)	2.04 (2)	2.8812 (15)	175 (2)
O3—H3B···O1^{iii}	0.76 (2)	2.16 (2)	2.9163 (16)	172 (2)

N1—H1C···O3^{iv}	0.90 (2)	1.97 (2)	2.8714 (18)	177.4 (17)
N1—H1A···O1^{ii}	0.87 (2)	2.40 (2)	3.1707 (18)	147.4 (17)
N1—H1B···O3^{v}	0.80 (2)	2.09 (2)	2.8891 (18)	170.5 (18)

Symmetry codes: (ii) $-x+2$, $-y+1$, $-z+1$; (iii) $x-1/2$, $y-1/2$, z; (iv) $-x+3/2$, $y+1/2$, $-z+1/2$; (v) x, $y+1$, z.

Fig. 1

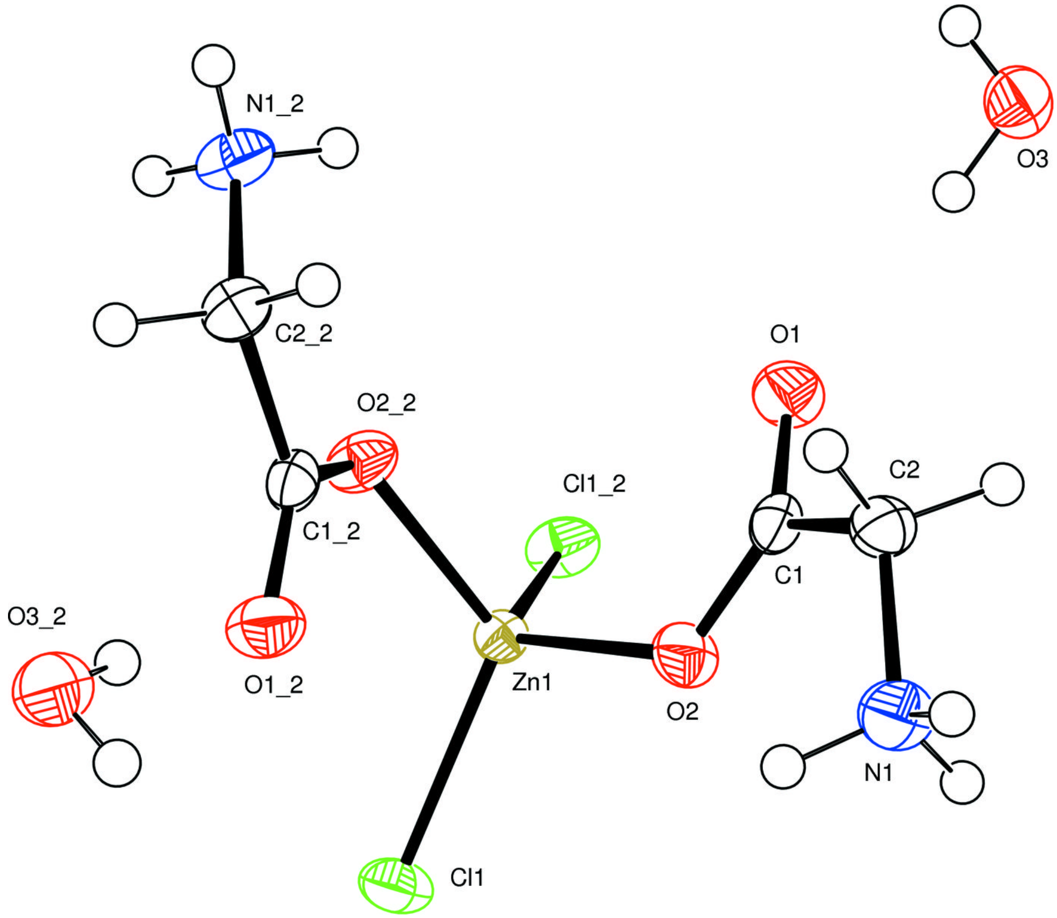

Fig. 2