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Dichlorobis(DL-alanine)zinc(II)

M. Subha Nandhini,[a] R. V. Krishnakumar[b] and S. Natarajan[a]*

[a]Department of Physics, Madurai Kamaraj University, Madurai 625 021, India, and [b]Department of Physics, Thiagarajar College, Madurai 625 009, India

Correspondence e-mail:
s_natarajan50@yahoo.com

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.005 Å
R factor = 0.040
wR factor = 0.114
Data-to-parameter ratio = 15.6

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

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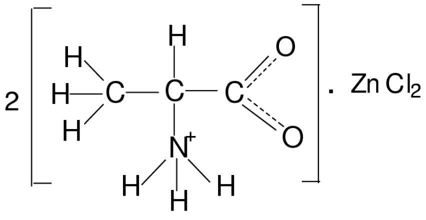
In the title compound, $[Zn(C_3H_7NO_2)_2Cl_2]$, both the alanine molecules in the asymmetric unit exist as zwitterions. Zn has a distorted tetrahedral coordination, with two Cl atoms and two O atoms, one from each of the two crystallographically independent alanine ligands in the asymmetric unit.

Comment

Halogenozinc–amino acid complexes are interesting, as zinc is known to compete successfully with cadmium for protein binding sites. Zinc also plays an important biological role in the formation of structural motifs called 'zinc fingers', which are characteristic of certain proteins that bind to DNA. The present study reports the crystal structure of a complex of DL-alanine with zinc chloride, namely dichlorobis(DL-alanine)-zinc(II). Alanine, a non-essential amino acid commonly present in proteins, is hydrophobic and non-polar. A precise determination of the crystal structure of DL-alanine itself was recently carried out in our laboratory (Subha Nandhini *et al.*, 2001*a*). The crystal structure of a complex of sarcosine with zinc chloride, trichloro(sarcosinio)zinc(II) monohydrate (Krishnakumar *et al.*, 2001), in which the amino acid exhibits an unusual cationic form, was also elucidated in our laboratory. A similar ionization state was observed in the case of the complex of L-histidine with zinc chloride (Forster *et al.*, 1993). The crystal structures of dichlorobis(sarcosinato)zinc(II) (Subha Nandhini *et al.*, 2001*b*) and dichlorobis(DL-valine)-zinc(II) (Subha Nandhini *et al.*, 2001*c*) have also been determined recently in our laboratory.



(I)

The molecular structure and atom-numbering scheme are shown in Fig. 1. Both the alanine molecules in the asymmetric unit, coordinating as ligands to Zn, exist as zwitterions. However, the C1—O1 and C1—O2 bond lengths in molecule *A* [1.265 (4) and 1.232 (4) Å, respectively] and molecule *B* [1.273 (4) and 1.230 (4) Å, respectively] show significant deviations from those usually exhibited by zwitterions. These deviations may be due to the fact that the O1 atoms of both molecule *A* and molecule *B* participate in the coordination

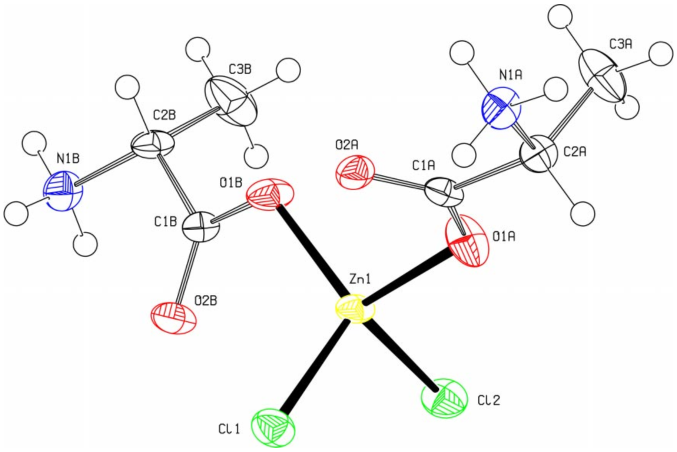


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are shown at the 50% probability level.

environment around Zn. The torsion angles O1*A*—Zn1—O1*B*—C1*B* [172.7 (2)°] and O1*B*—Zn1—O1*A*—C1*A* [69.1 (3)°] describe the relative orientation of molecules *A* and *B* with respect to the metal. The coordination environment around Zn is remarkably similar to those observed in the structures of the complex of $ZnCl_2$ with sarcosine (Subha Nandhini *et al.*, 2001*b*), glycine (Hariharan *et al.*, 1989) and L-proline (Yukawa *et al.*, 1985). Fig. 2 shows the packing of the molecules of (I), viewed down the *b* axis. The molecules aggregate into a layered arrangement parallel to the *bc* plane. These layers form hydrogen-bonded double layers involving inversion- and glide-related molecules. Adjacent double layers have no hydrogen-bonded interactions between them and are held together by van der Waals interactions.

Experimental

Colourless single crystals of (I) were grown as transparent plates by slow evaporation of a saturated water–acetone mixture containing DL-alanine and zinc chloride, in the stoichiometric ratio of 1:1.

Crystal data

$[Zn(C_3H_7NO_2)_2Cl_2]$
$M_r = 314.46$
Monoclinic, $P2_1/c$
$a = 9.996\ (5)$ Å
$b = 13.622\ (4)$ Å
$c = 8.616\ (3)$ Å
$\beta = 90.30\ (1)°$
$V = 1173.2\ (8)$ Å^3
$Z = 4$
$D_x = 1.780$ Mg m^{-3}
$D_m = 1.77\ (2)$ Mg m^{-3}
D_m measured by flotation in a liquid mixture of carbon tetrachloride and bromoform
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 16–24°$
$\mu = 7.12$ mm^{-1}
$T = 293\ (2)$ K
Plates, colourless
0.20 × 0.14 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scans (North *et al.*, 1968)
$T_{min} = 0.35$, $T_{max} = 0.49$
2282 measured reflections
2134 independent reflections
2097 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 67.9°$
$h = -12 \rightarrow 11$
$k = -16 \rightarrow 0$
$l = 0 \rightarrow 10$
2 standard reflections every 100 reflections intensity decay: <1%

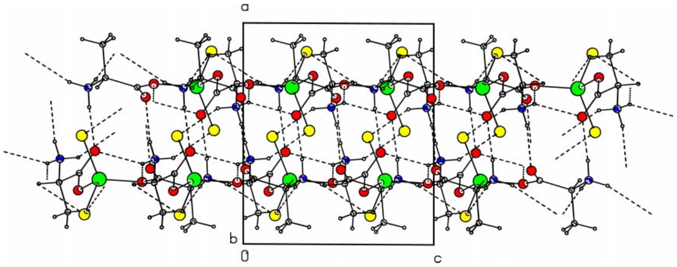


Figure 2
Packing diagram of (I), viewed down the *b* axis.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.114$
$S = 1.15$
2134 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0605P)^2 + 2.8047P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.51$ e Å^{-3}
$\Delta\rho_{min} = -0.96$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0030 (4)

Table 1
Selected geometric parameters (Å, °).

Zn1—O1*A*	1.967 (3)	C1*A*—C2*A*	1.531 (4)
Zn1—O1*B*	1.990 (3)	C2*A*—C3*A*	1.513 (6)
Zn1—Cl2	2.2572 (11)	O1*B*—C1*B*	1.273 (4)
Zn1—Cl1	2.2599 (13)	O2*B*—C1*B*	1.230 (4)
O2*A*—C1*A*	1.232 (4)	C1*B*—C2*B*	1.518 (4)
O1*A*—C1*A*	1.265 (4)	C2*B*—C3*B*	1.523 (6)
O1*A*—Zn1—O1*B*	106.06 (12)	O1*A*—Zn1—Cl1	110.20 (9)
O1*A*—Zn1—Cl2	102.53 (9)	O1*B*—Zn1—Cl1	117.77 (9)
O1*B*—Zn1—Cl2	112.45 (8)	Cl2—Zn1—Cl1	106.78 (5)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*1···O2*B*^{i}	0.89	2.15	2.864 (4)	137
N1*A*—H1*A*2···Cl1^{i}	0.89	2.39	3.204 (3)	152
N1*A*—H1*A*3···O1*B*^{ii}	0.89	2.22	2.960 (4)	141
N1*B*—H1*B*1···Cl2^{iii}	0.89	2.62	3.478 (3)	163
N1*B*—H1*B*2···O2*A*^{iv}	0.89	2.00	2.886 (4)	172
N1*B*—H1*B*3···Cl2^{v}	0.89	2.43	3.317 (3)	173
C2*B*—H2*B*···Cl1^{iv}	0.98	2.77	3.680 (4)	154

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

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1990); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 1999); software used to prepare material for publication: *SHELXL*97.

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