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Dichlorobis(sarcosinato)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: xray@mrna.tn.nic.in

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Key indicators

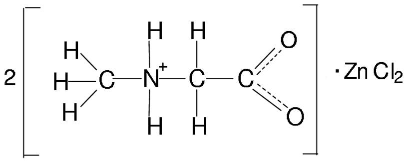
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.004 Å
R factor = 0.028
wR factor = 0.075
Data-to-parameter ratio = 15.9

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

In the title compound, [$ZnCl_2(CH_3NH_2{}^+CH_2COO^-)_2$], the sarcosine ligand coordinates to the metal in the zwitterionic form. The Zn atom has a distorted tetrahedral coordination with two Cl atoms and two O atoms, one each from the two crystallographically independent sarcosine molecules in the asymmetric unit. Head-to-tail hydrogen bonds between the amino acid molecules, in addition to N—H···Cl, C—H···O and C—H···Cl hydrogen bonds, stabilize the packing of the molecules.

Comment

Sarcosine (*N*-methylglycine, $CH_3NH_2{}^+CH_2COO^-$), an intermediate in the metabolism of choline, occurs naturally in large amounts in starfish and sea urchins. The crystal structure of sarcosine itself was previously determined in our laboratory (Mostad & Natarajan, 1989). Zinc–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 a structural motif called zinc fingers which are characteristic of certain proteins that bind to DNA. Recently, the crystal structure of a complex of sarcosine with zinc chloride, namely trichloro(sarcosinio)zinc(II) monohydrate (Krishnakumar *et al.*, 2001), in which the amino acid exhibits an unusual cationic form, was reported. The present work reports the crystal structure of a complex, (I), of sarcosine with zinc chloride where the amino acid adopts the usually expected zwitterionic form. The crystal structures of complexes of $ZnCl_2$ with glycine (Hariharan *et al.*, 1989), L-proline (Yukawa *et al.*, 1985) and L-histidine (Foster *et al.*, 1993) have already been reported.



(I)

In Fig. 1, the molecular structure and atom-numbering scheme are shown. Both the sarcosine molecules in the asymmetric unit exist as zwitterions, each with a positively charged amino group and a negatively charged carboxylate group. However, the C1—O1 and C1—O2 bond lengths in molecule *A* [1.276 (3) and 1.223 (3) Å, respectively] and molecule *B* [1.261 (3) and 1.213 (3) Å, respectively] show significant deviations from those usually exhibited by a zwitterion. The larger value observed in the C1—O1 bond lengths may be due to the fact that both the O1 atoms of molecule *A* and *B* participate in the coordination environment around the metal. The angle between the planes formed by the atoms of the two sarcosine molecules coordinating to Zn is 81.5 (1)°.

Zinc is known to have both tetrahedral and octahedral coordination in crystal structures (Cingi *et al.*, 1972). In the present structure, zinc has a distorted tetrahedral environment with two Cl atoms and two carboxyl O atoms, one each from the two crystallographically independent sarcosine molecules in the asymmetric unit. The angles around the Zn atom range from 101.36 (5) to 115.74 (3)°. The coordination environment around Zn in trichloro(sarcosinio)zinc(II) monohydrate, however, is different since it involves three chlorines and one of the carboxyl O atoms.

Head-to-tail hydrogen bonds between the amino acid molecules, in addition to N—H···Cl, C—H···O and C—H···Cl hydrogen bonds, stabilize the three-dimensional network of the molecules. The crystal structure of (I) does not bear any relation either to that of trichloro(sarcosinio)zinc(II) monohydrate or to those of sarcosine cadmium chloride (Krishnakumar *et al.*, 1996) and sarcosine barium chloride tetrahydrate (Krishnakumar & Natarajan, 1995). However, the unit-cell parameters of (I) and those of sarcosine barium chloride tetrahydrate bear an interesting relationship as the *b* and *c* axes are very nearly equal and the cell length *a* in (I) is twice that of the other.

Experimental

Colorless single crystals of (I) were grown as transparent needles from a saturated water–acetone mixture containing sarcosine and zinc chloride in a 1:1 stoichiometric ratio.

Crystal data

$[ZnCl_2(C_6H_{14}N_2O_4)]$
$M_r = 314.46$
Orthorhombic, *Pbca*
$a = 14.191$ (2) Å
$b = 10.655$ (1) Å
$c = 15.917$ (2) Å
$V = 2406.5$ (4) Å^3
$Z = 8$
$D_x = 1.736$ Mg m^{-3}
$D_m = 1.74$ Mg m^{-3}
D_m measured by flotation in a mixture of carbon tetrachloride and bromoform
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 15$–27°
$\mu = 6.94$ mm^{-1}
$T = 293$ (2) K
Needle, colorless
0.16 × 0.12 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω–2θ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{\min} = 0.400$, $T_{\max} = 0.503$
2182 measured reflections
2182 independent reflections
2004 reflections with $I > 2\sigma(I)$
$\theta_{\max} = 67.9°$
$h = 0 \rightarrow 16$
$k = 0 \rightarrow 12$
$l = 0 \rightarrow 19$
2 standard reflections every 200 reflections
intensity decay: 0.1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.028$
$wR(F^2) = 0.075$
$S = 1.18$
2182 reflections
137 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0299P)^2 + 2.1069P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.28$ e Å^{-3}
$\Delta\rho_{\min} = -0.43$ e Å^{-3}
Extinction correction: *SHELXL*97
Extinction coefficient: 0.00071 (4)

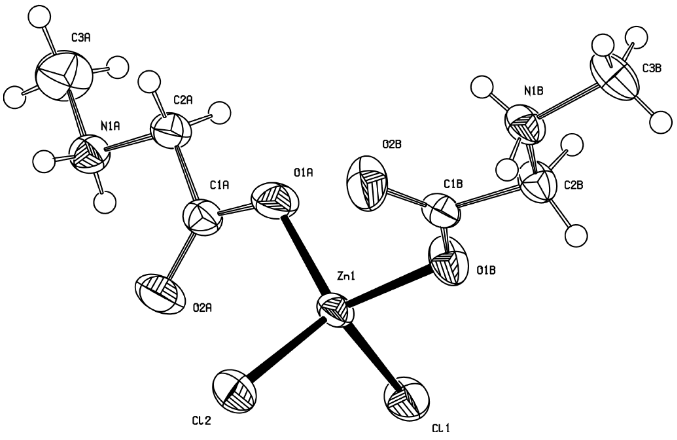


Figure 1
The structure of (I) with 50% probability displacement ellipsoids.

Table 1
Selected geometric parameters (Å, °).

Zn1—O1*A*	1.9484 (19)	O2*B*—C1*B*	1.213 (3)
Zn1—O1*B*	1.9713 (17)	N1*A*—C2*A*	1.471 (3)
Zn1—Cl2	2.2595 (7)	N1*A*—C3*A*	1.484 (3)
Zn1—Cl1	2.2739 (7)	N1*B*—C3*B*	1.478 (3)
O1*A*—C1*A*	1.276 (3)	N1*B*—C2*B*	1.479 (3)
O1*B*—C1*B*	1.261 (3)	C1*A*—C2*A*	1.514 (3)
O2*A*—C1*A*	1.223 (3)	C1*B*—C2*B*	1.519 (3)
O1*A*—Zn1—O1*B*	107.20 (8)	O2*A*—C1*A*—O1*A*	126.6 (2)
O1*A*—Zn1—Cl2	113.40 (6)	O2*A*—C1*A*—C2*A*	120.0 (2)
O1*B*—Zn1—Cl2	111.71 (6)	O1*A*—C1*A*—C2*A*	113.4 (2)
O1*A*—Zn1—Cl1	106.43 (6)	O2*B*—C1*B*—O1*B*	127.0 (2)
O1*B*—Zn1—Cl1	101.36 (5)	O2*B*—C1*B*—C2*B*	119.3 (2)
Cl2—Zn1—Cl1	115.74 (3)	O1*B*—C1*B*—C2*B*	113.7 (2)
C2*A*—N1*A*—C3*A*	113.9 (2)	N1*A*—C2*A*—C1*A*	111.4 (2)
C3*B*—N1*B*—C2*B*	112.97 (19)	N1*B*—C2*B*—C1*B*	111.88 (19)
C3*A*—N1*A*—C2*A*—C1*A*	−171.6 (2)	C3*B*—N1*B*—C2*B*—C1*B*	−166.3 (2)
O2*A*—C1*A*—C2*A*—N1*A*	−1.3 (3)	O2*B*—C1*B*—C2*B*—N1*B*	2.1 (3)
O1*A*—C1*A*—C2*A*—N1*A*	178.0 (2)	O1*B*—C1*B*—C2*B*—N1*B*	−179.2 (2)

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}	0.90	1.93	2.714 (3)	144
N1*A*—H1*A*2···Cl1^{ii}	0.90	2.35	3.223 (2)	163
N1*B*—H1*B*1···Cl2^{iii}	0.90	2.42	3.291 (2)	164
N1*B*—H1*B*2···Cl2^{iv}	0.90	2.44	3.191 (2)	141
N1*B*—H1*B*2···O2*A*^{iii}	0.90	2.48	2.985 (3)	116
C2*A*—H2*A*2···O1*B*^{v}	0.97	2.40	3.342 (3)	164
C2B—H2*B*2···Cl1^{vi}	0.97	2.76	3.610 (3)	146
C3*A*—H3*A*1···O2*A*^{ii}	0.96	2.66	3.555 (4)	156

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

The H atoms were placed in calculated positions and were allowed to ride on their respective parent atoms using *SHELXL*97 (Sheldrick, 1997) defaults.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *CAD*-4 *Software*;

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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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