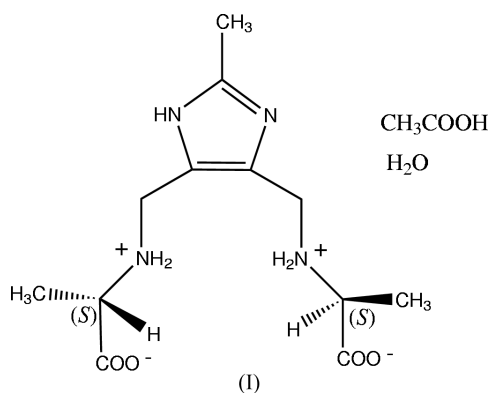


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Key indicators

Single-crystal X-ray study
T = 298 K
Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
R factor = 0.041
wR factor = 0.117
Data-to-parameter ratio = 12.2For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.4,4'-(2-Methyl-1*H*-imidazole-4,5-diyl)bis[2(*S*)-
methyl-3-azoniabutanoate] acetic acid monohydrateIn the title compound, $\text{C}_{12}\text{H}_{20}\text{N}_4\text{O}_4 \cdot \text{C}_2\text{H}_4\text{O}_2 \cdot \text{H}_2\text{O}$, the main fragment contains two L-alanine residues with a zwitterionic structure. The crystal structure is characterized by a two-dimensional network of $\text{O}-\text{H} \cdots \text{O}$, $\text{O}-\text{H} \cdots \text{N}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds.

Comment

The preparation and characterization of imidazole derivatives is of current interest, because of their ability to form metal complexes with a wide variety of chemical, magnetic and catalytic properties (Baesjou *et al.*, 1998; Colacio *et al.*, 2000; Kamaraj *et al.*, 2003). In previous work (Mendoza-Díaz *et al.*, 1996, 2002), we have reported the synthesis and crystal structures of ligands obtained *via* the Mannich addition of primary amines on 2-methylimidazole, to give a ten-membered cyclic diazecine, incorporating two imidazoles and two amines. Following this line of research, we now describe a non-cyclic ligand, (I), obtained from a similar reaction between 2-methylimidazole and L-alanine, and crystallized with acetic acid and water.The asymmetric unit of (I) consists of a zwitterion of formula $\text{C}_{12}\text{H}_{20}\text{N}_4\text{O}_4$, an acetic acid molecule and a water molecule. The main molecule contains two alanine groups bonded, *via* two methylene groups, to positions 4 and 5 of a 2-methylimidazole group (Fig. 1). The geometry of the imidazole ring is as expected (Table 1), with $\text{C}=\text{C}$ and $\text{C}=\text{N}$ bond lengths ranging from 1.329 (3) to 1.378 (3) \AA . Atom H1 is clearly bonded to N1, and no evidence can be found, at least in the solid state, for a tautomerism in this heterocycle. The imidazole group thus has potential for coordination through atom N3. Both alanine groups have zwitterionic structures, with both carboxylate groups having similar $\text{C}=\text{O}$ bond lengths [1.231 (3)–1.259 (3) \AA] and protonated amine groups displaying characteristic $\text{C}-\text{N}$ single bond lengths of around

Received 16 December 2004

Accepted 4 January 2005

Online 15 January 2005

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.117$
 $S = 1.03$
 3107 reflections
 254 parameters
 H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0655P)^2 + 0.0268P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.0001$
 $\Delta\rho_{\max} = 0.22 \text{ e } \text{Å}^{-3}$
 $\Delta\rho_{\min} = -0.21 \text{ e } \text{Å}^{-3}$

Table 1

Selected geometric parameters (Å, °).

N1—C2	1.332 (3)	C10—O12	1.238 (2)
N1—C5	1.374 (3)	C14—N15	1.499 (3)
C2—N3	1.329 (3)	N15—C16	1.499 (2)
N3—C4	1.378 (3)	C17—O18	1.231 (3)
C7—N8	1.502 (3)	C17—O19	1.255 (3)
N8—C9	1.497 (3)	C22—O24	1.212 (3)
C10—O11	1.259 (3)	C22—O23	1.280 (4)
O12—C10—O11	127.25 (18)	O19—C17—C16	115.4 (2)
O12—C10—C9	119.45 (19)	O24—C22—O23	123.0 (3)
O11—C10—C9	113.26 (16)	O24—C22—C21	120.7 (3)
O18—C17—O19	125.5 (2)	O23—C22—C21	116.3 (3)
O18—C17—C16	119.05 (17)		

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
O23—H3 ⁱ ···N3	1.06 (3)	1.51 (3)	2.569 (3)	177 (3)
N8—H8a ⁱ ···O25	0.94 (3)	1.90 (3)	2.823 (2)	170 (3)
N15—H15a ⁱ ···O25	0.89 (3)	1.97 (3)	2.817 (2)	159 (3)
N15—H15b ⁱ ···O24	0.93 (3)	1.90 (3)	2.832 (3)	174 (3)
N1—H1 ⁱ ···O11 ⁱ	0.90 (3)	1.70 (3)	2.585 (2)	168 (4)
N8—H8b ⁱ ···O12 ⁱ	0.99 (3)	1.85 (3)	2.815 (2)	167 (3)
O25—H251 ⁱⁱ ···O19 ⁱⁱⁱ	0.87 (4)	1.78 (4)	2.636 (3)	169 (3)
O25—H252 ⁱ ···O18 ⁱⁱⁱ	0.85 (4)	1.99 (4)	2.838 (2)	172 (3)
O25—H252 ⁱ ···O19 ⁱⁱⁱ	0.85 (4)	2.42 (4)	3.027 (3)	129 (3)

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

In the absence of significant anomalous scattering effects, Friedel pairs were merged. The absolute configuration of (I) was assigned on

the basis of the known configuration of the L-alanine used as starting material. H atoms bonded to C atoms were placed at idealized positions and refined using a riding model, with $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{parent C atom})$. The constrained distances and x parameters are the default values in *SHELXTL-Plus* (Sheldrick, 1998): methine: C—H = 0.98 Å, $x = 1.2$; methylene: C—H = 0.97 Å, $x = 1.2$; methyl: C—H = 0.96 Å, $x = 1.5$. Other H atoms were found in difference maps and refined with free coordinates and fixed isotropic displacement parameters [$U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{parent atom})$]. In the case of H3, atom N3 [$U_{\text{eq}} = 0.046 (1) \text{ Å}^2$] was chosen as parent atom rather than O23 [$U_{\text{eq}} = 0.104 (1) \text{ Å}^2$]. Refinement attempts with O23 as parent atom for H3 resulted in an O23—H3 bond length of 1.15 (6) Å, while the present refinement yields O23—H3 = 1.06 (3) Å, which seems to be more reasonable for a hydroxy group. This atom H has been labeled H3 even though formally belonging to the acetate group.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXTL-Plus* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus* and *MERCURY* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXTL-Plus*.

LG thanks CONACyT (grant No. 34847-E) for financial support.

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