

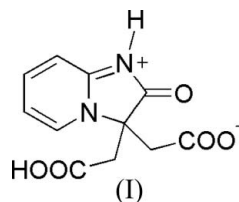
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Key indicators

Single-crystal X-ray study
 $T = 293$ K
Mean $\sigma(\text{C}-\text{C}) = 0.002$ Å
 R factor = 0.063
 wR factor = 0.162
Data-to-parameter ratio = 18.1For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Zwitterionic 3-carboxylatomethyl-3-carboxymethyl-
2-oxo-2,3-dihydroimidazo[1,2-*a*]pyridin-1-iumThe title compound, $\text{C}_{11}\text{H}_{10}\text{N}_2\text{O}_5$, exists in the solid state as a
carboxylate–imidazolium zwitterion. Intermolecular $\text{O}-\text{H}\cdots\text{O}$
and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds link the molecules
into two-dimensional layers.Received 19 August 2006
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Comment

Imidazo[1,2-*a*]pyridine derivatives are important inter-
mediates in organic synthesis (Baumann *et al.*, 1984), espe-
cially in the synthesis of biologically active and medicinally
useful agents. For instance, they are widely used in the
synthesis of cyclin-dependent kinase (CDK) inhibitors
(Anderson *et al.*, 2003), sleep inducers (Hempel & Blaschke,
1996), anticonvulsant agents (Trapani *et al.*, 2003) and antiviral
agents (Gueiffier *et al.*, 1998; Mavel *et al.*, 2002). We have
exploited a new and convenient method to obtain the title
compound, (I), which was prepared from the reaction of
potassium chloroacetate with 2-aminopyridine in aqueous
alkaline solution.In the solid state, (I) exhibits a zwitterionic form (Fig. 1).
Each zwitterionic molecule acts as T-shaped connector,
forming hydrogen bonds to three other molecules. The
carboxyl groups link to two other molecules through $\text{O}-\text{H}\cdots\text{O}$
hydrogen bonds (Table 1) to form chains extending
along the *c* direction. The NH group of the imidazolium ring
links these chains *via* $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Table 1) to
form layers in the *bc* plane (Fig. 2). Between adjacent layers,
the pyridine rings form $\pi-\pi$ stacking contacts, with an inter-
planar separation of 3.50 (1) Å and a centroid–centroid
distance of 4.03 (1) Å.

Experimental

A solution of KOH (0.6 mol, 33.6 g) in 75 ml of water was added
dropwise to a solution of chloroacetic acid (0.3 mol, 28.4 g) in 75 ml
of water cooled in an ice bath. To the resulting alkaline solution, 2-
aminopyridine (0.1 mol, 9.4 g) was added slowly, and the mixture was
refluxed at 359 K for 30 h. 6 *N* HCl (53 ml) was added to neutralize
the solution, which was then concentrated by boiling and cooled in an
ice bath to remove KCl. After the mother liquor (pH 2–3) had been
allowed to stand in a refrigerator for three days, the desired acid was

separated out and collected by filtration. The solid was recrystallized in a hot ethanol–water (1:1) mixture, and the colourless product was collected by filtration and air-dried (yield 23%). Block-shaped crystals of (I) suitable for X-ray diffraction analysis were obtained by slow evaporation of a DMF/H₂O (1:1) solution.

Crystal data

C ₁₁ H ₁₀ N ₂ O ₅	Z = 8
M _r = 250.21	D _x = 1.437 Mg m ⁻³
Monoclinic, C2/c	Mo K α radiation
a = 13.735 (3) Å	μ = 0.12 mm ⁻¹
b = 9.862 (2) Å	T = 293 (2) K
c = 18.218 (4) Å	Block, colourless
β = 110.35 (3)°	0.40 × 0.36 × 0.27 mm
V = 2313.7 (10) Å ³	

Data collection

Siemens SMART CCD diffractometer	11493 measured reflections
φ and ω scans	3040 independent reflections
Absorption correction: multi-scan (SADABS; Bruker, 1998)	2852 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.955$, $T_{\max} = 0.969$	$R_{\text{int}} = 0.050$
	$\theta_{\text{max}} = 29.7^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0914P)^2 + 1.0573P]$
$R[F^2 > 2\sigma(F^2)] = 0.063$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.162$	$(\Delta/\sigma)_{\text{max}} < 0.001$
S = 1.13	$\Delta\rho_{\text{max}} = 0.75 \text{ e \AA}^{-3}$
3040 reflections	$\Delta\rho_{\text{min}} = -0.69 \text{ e \AA}^{-3}$
168 parameters	Extinction correction: SHELXL97
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.030 (3)

Table 1

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
O3—H3...O1 ⁱ	1.12 (3)	1.39 (3)	2.4724 (16)	162 (3)
N1—H1...O2 ⁱⁱ	0.86	2.03	2.7734 (16)	145

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

H atoms bound to C atoms were placed in calculated positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å, and with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. Atom H1, attached to N1, was also placed geometrically, with N—H = 0.86 Å and allowed to ride with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. Atom H3, attached to O3, was located in a difference Fourier map and refined isotropically without restraint.

Data collection: SMART (Bruker, 1998); cell refinement: SAINT (Bruker, 1998); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Bruker, 1998); software used to prepare material for publication: SHELXTL.

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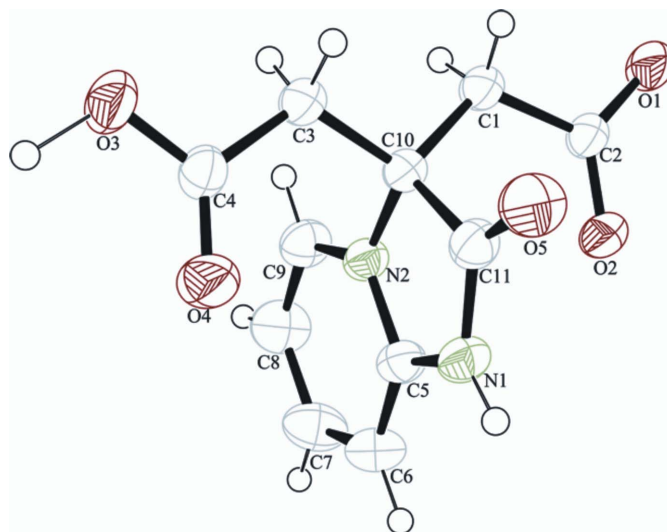


Figure 1

The molecular structure of (I), with displacement ellipsoids shown at the 50% probability level for non-H atoms.

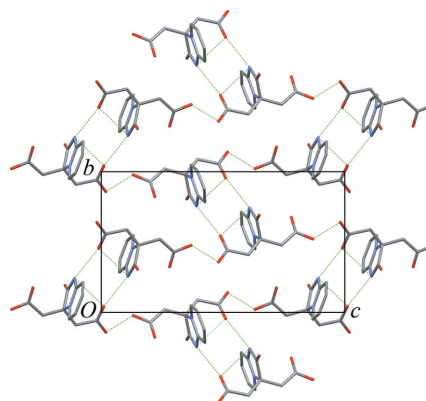


Figure 2

Projection along a showing a single layer of molecules in the bc plane, linked by O—H...O and N—H...O hydrogen bonds (dashed lines). H atoms are omitted.

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