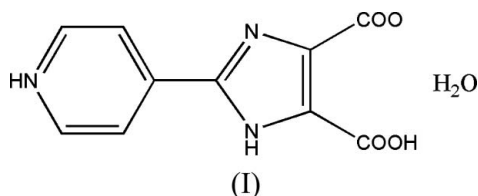


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Key indicators

Single-crystal X-ray study
 $T = 298$ K
Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å
 R factor = 0.051
 wR factor = 0.111
Data-to-parameter ratio = 11.7For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.The inner salt 4-carboxy-2-(pyridinium-4-yl)-
1*H*-imidazole-5-carboxylate monohydrateIn the title compound, $\text{C}_{10}\text{H}_7\text{N}_3\text{O}_4 \cdot \text{H}_2\text{O}$, one carboxyl group is
deprotonated and the pyridyl group is protonated. The inner
salt molecule has a planar structure, apart from the carboxylic
acid group, which is tilted from the imidazole plane by a small
dihedral angle of 7.3 (3)°.Received 9 May 2006
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Comment

Imidazole-4,5-dicarboxylate has been used to prepare metal
complex polymers (Lu *et al.*, 2006). Recently, we prepared the
title compound, (I), and we present its crystal structure here.The molecular structure of (I) is shown in Fig. 1. The C1-
containing carboxyl group is deprotonated (Table 1) and
forms an intramolecular hydrogen bond with the neighboring
C4-containing carboxyl group. The molecule displays a planar
structure, apart from the C4-carboxyl group, which is tilted
from the imidazole plane by a small dihedral angle of 7.3 (3)°.Intermolecular $\text{O}-\text{H} \cdots \text{O}$ and $\text{N}-\text{H} \cdots \text{O}$ hydrogen
bonding occurs (Table 2), helping to stabilize the crystal
structure.

Experimental

2-(4-Pyridyl)benzimidazole (1 g, 5.13 mmol) was prepared in accor-
dance with the literature method (Alcalde *et al.*, 1992), and was then
added to 98% H_2SO_4 (8.4 ml) in portions. An H_2O_2 solution (30%,
8 ml) was added dropwise to the above solution at 373 K. The
resulting solution was then stirred for 1 h at 413 K. After cooling to
313 K, water (200 ml) was added. The precipitated product was
filtered off, washed with water and dried, yielding a light-yellow
powder (0.68 g). A suspension of the yellow powder (5 mg,
0.02 mmol) in water (2 ml) was sealed in a 6 ml glass tube and heated
at 423 K for 3 d, then cooled to room temperature to obtain suitable
single crystals of (I).

Crystal data

 $\text{C}_{10}\text{H}_7\text{N}_3\text{O}_4 \cdot \text{H}_2\text{O}$
 $M_r = 251.20$
Monoclinic, $P2_1/c$
 $a = 5.6348$ (15) Å
 $b = 8.457$ (2) Å
 $c = 21.605$ (6) Å
 $\beta = 94.889$ (4)°
 $V = 1025.7$ (5) Å³ $Z = 4$
 $D_x = 1.627$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.13$ mm⁻¹
 $T = 298$ (2) K
Platelet, yellow
 $0.26 \times 0.24 \times 0.03$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.966$, $T_{\max} = 0.990$

5216 measured reflections
 1912 independent reflections
 1541 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.034$
 $\theta_{\text{max}} = 25.5^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.051$
 $wR(F^2) = 0.111$
 $S = 1.12$
 1912 reflections
 163 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0437P)^2 + 0.2198P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.24 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.23 \text{ e } \text{\AA}^{-3}$

Table 1

Selected bond lengths (Å).

C1—O3	1.270 (3)	C4—O1	1.213 (3)
C1—O4	1.230 (3)	C4—O2	1.300 (3)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N1—H1N \cdots O5 ⁱ	0.98	1.80	2.758 (2)	164
N3—H3N \cdots O4 ⁱⁱ	0.94	1.84	2.779 (2)	174
O2—H2A \cdots O3	0.96	1.51	2.462 (2)	173
O5—H5B \cdots O1 ⁱⁱⁱ	0.90	1.90	2.759 (2)	161
O5—H5A \cdots O3 ^{iv}	0.88	1.90	2.768 (2)	172

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

H atoms attached to N and O atoms were located in a difference Fourier map and refined as riding in their as-found relative positions, with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O,N})$. Other H atoms were placed in calculated positions with $C-H = 0.93 \text{ \AA}$ and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{iso}}(\text{C})$.

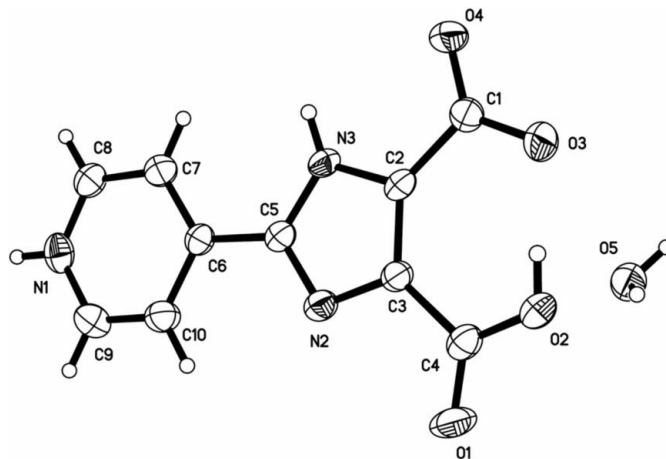


Figure 1

The molecular structure of (I), with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); 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, 2000); software used to prepare material for publication: SHELXTL.

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