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## Key indicators

Single-crystal X-ray study  
 $T = 295$  K  
Mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å  
 $R$  factor = 0.036  
 $wR$  factor = 0.100  
Data-to-parameter ratio = 14.8For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

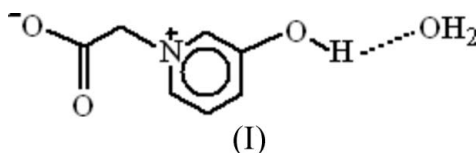
## 3-Hydroxypyridinium-1-acetate monohydrate

In the betaine title compound,  $\text{C}_7\text{H}_7\text{NO}_3 \cdot \text{H}_2\text{O}$  or  $\text{HOC}_5\text{H}_4\text{N}^+\text{CH}_2\text{CO}_2^-\cdot\text{H}_2\text{O}$ , 3-hydroxypyridinium-1-acetate interacts with the water molecule to form a two-dimensional hydrogen-bonded framework.

## Comment

Pyridinioacetate,  $\text{C}_5\text{H}_5\text{N}^+-\text{CH}_2\text{CO}_2^-$ , is a zwitterionic compound that yields a number of adducts with metal salts (Yang *et al.*, 2003). Our studies have been concerned with the solid-state structure of hydroxy-substituted pyridinioacetate and directed toward the synthesis of metal salts (Gao, Huo *et al.*, 2004; Gao, Zhang *et al.*, 2004; Zhang *et al.*, 2004*a,b*). 3-Hydroxypyridinium-1-acetic acid cocrystallizes with 1-carboxymethyl-3-hydroxypyridinium chloride (1/1) (Zhao *et al.*, 2004), the cation interacting with the zwitterion.

In this paper, we report the structure of the zwitterionic title compound, (I). The O1—C7 and O2—C7 bond lengths are 1.2440 (16) Å and 1.2375 (16) Å, indicating electron delocalization (Table 1). The carboxylate group O1—C7—O2 is twisted out of the attached pyridine ring plane, the dihedral angle being 66.1 (3)°. The water molecule interacts with the O atoms of the hydroxy and carboxylate groups (Table 2), giving rise to a two-dimensional hydrogen-bonded framework (Fig. 2).



## Experimental

Cadmium dinitrate tetrahydrate (3.08 g, 10 mmol) and imidazole (0.69 g, 10 mmol) were added to an aqueous solution of 1-carboxymethyl-3-hydroxypyridinium chloride–3-hydroxypyridinium-1-acetate (1/1) (3.43 g, 10 mmol). The mixture was stirred for 0.5 h and then filtered. Colorless crystals of the title compound separated from the solution after several days. Analysis calculated for  $\text{C}_7\text{H}_9\text{NO}_4$ : C 49.12, H 5.30, N 8.18%; found: C 49.16, H 5.34, N 8.16%.

## Crystal data

$\text{C}_7\text{H}_7\text{NO}_3 \cdot \text{H}_2\text{O}$   
 $M_r = 171.15$   
Orthorhombic, *Pbca*  
 $a = 8.8417$  (18) Å  
 $b = 12.081$  (2) Å  
 $c = 14.262$  (3) Å  
 $V = 1523.5$  (5) Å<sup>3</sup>  
 $Z = 8$   
 $D_x = 1.492$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation  
Cell parameters from 11630  
reflections  
 $\theta = 3.2$ – $27.4^\circ$   
 $\mu = 0.12$  mm<sup>-1</sup>  
 $T = 295$  (2) K  
Thick plate, colorless  
 $0.39 \times 0.26 \times 0.15$  mm

## Data collection

Rigaku R-AXIS RAPID  
diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan  
(*ABSCOR*; Higashi, 1995)  
 $T_{\min} = 0.962$ ,  $T_{\max} = 0.982$   
13670 measured reflections

1742 independent reflections  
1459 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$   
 $\theta_{\text{max}} = 27.5^\circ$   
 $h = -10 \rightarrow 11$   
 $k = -15 \rightarrow 15$   
 $l = -18 \rightarrow 18$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.100$   
 $S = 1.03$   
1742 reflections  
118 parameters  
H atoms treated by a mixture of  
independent and constrained  
refinement

$w = 1/[\sigma^2(F_o^2) + (0.0526P)^2 + 0.3906P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} < 0.001$   
 $\Delta\rho_{\text{max}} = 0.24 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.17 \text{ e } \text{\AA}^{-3}$

Table 1

Selected geometric parameters ( $\text{\AA}$ ,  $^\circ$ ).

N1—C5	1.3423 (17)	C1—C2	1.3847 (18)
N1—C1	1.3424 (16)	C2—C3	1.3890 (18)
N1—C6	1.4741 (16)	C3—C4	1.382 (2)
O1—C7	1.2440 (16)	C4—C5	1.368 (2)
O2—C7	1.2375 (16)	C6—C7	1.5392 (18)
O3—C2	1.3348 (16)		
N1—C1—C2	120.27 (11)	O3—C2—C3	124.77 (12)
N1—C5—C4	119.64 (12)	C1—N1—C6	118.89 (11)
N1—C6—C7	112.88 (10)	C1—C2—C3	118.75 (12)
O1—C7—C6	114.52 (11)	C4—C3—C2	119.13 (12)
O2—C7—O1	127.42 (12)	C5—N1—C1	121.85 (11)
O2—C7—C6	117.97 (11)	C5—N1—C6	119.09 (11)
O3—C2—C1	116.48 (12)	C5—C4—C3	120.34 (13)

Table 2

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1W—H1W1 $\cdots$ O2 <sup>i</sup>	0.86 (1)	1.86 (1)	2.6934 (14)	165 (2)
O1W—H1W2 $\cdots$ O1 <sup>ii</sup>	0.85 (1)	1.85 (1)	2.6980 (15)	170 (2)
O3—H7 $\cdots$ O1W	0.87 (1)	1.70 (1)	2.5627 (15)	171 (2)

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

The H atoms attached to O atoms were located in a difference map and refined with O—H and H $\cdots$ H distances restrained to 0.85 (1) and 1.39 (1)  $\text{\AA}$ , respectively;  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{O})$ . All other H atoms were placed in calculated positions, with aromatic C—H = 0.93  $\text{\AA}$  and aliphatic C—H = 0.97  $\text{\AA}$ , and were included in the refinement in the riding-model approximation, with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

Data collection: *RAPID-AUTO* (Rigaku Corporation, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MS, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

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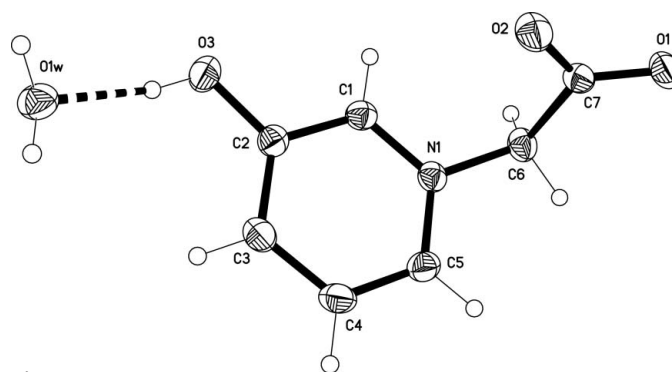


Figure 1

The atom-numbering scheme and displacement ellipsoids at the 50% probability level. An intermolecular hydrogen bond is shown as a dashed line.

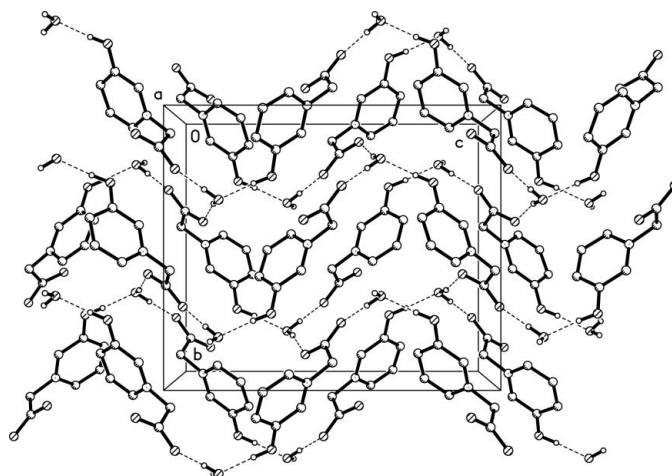


Figure 2

A plot of the hydrogen-bonding (dashed lines) network of (I). H atoms not involved in hydrogen bonding have been omitted.

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