

2-Amino-6-methylpyridinium 2-formylbenzoate
monohydrateOrhan Büyükgüngör^a and
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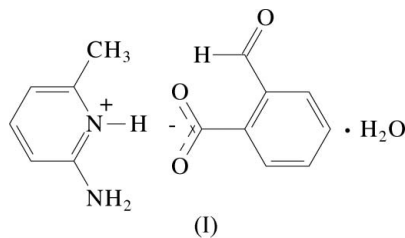
Key indicators

Single-crystal X-ray study
T = 296 K
Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
R factor = 0.041
wR factor = 0.117
Data-to-parameter ratio = 12.1For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, $\text{C}_6\text{H}_9\text{N}_2^+ \cdot \text{C}_8\text{H}_5\text{O}_3^- \cdot \text{H}_2\text{O}$, contains hydrogen-bonded $[\text{R}_2^2(8)\text{R}_4^2(8)\text{R}_2^2(8)]$ motifs involving 2-amino-6-methylpyridinium and 2-carboxylbenzoate ions. These motifs are connected by three $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds involving two water O atoms.

Comment

The title compound was obtained by the reaction of 2-amino-6-methylpyridine and 2-formylbenzoic acid. The copper(II) complexes of 2-aminopyridinium carboxylates have important properties in the applications in pharmaceuticals, fungicides, oxygen transfer, oxidative addition, homogenous hydrogenation, gas occlusion compounds and solvent extraction processes (Lah *et al.*, 2001; Yang *et al.*, 1995). Intermolecular interaction analyses in crystalline systems are very important in supramolecular chemistry, which can be defined as the chemistry (Braga *et al.*, 2002). These interactions are responsible for crystal packing, and through an understanding of such interactions we can comprehend collective properties and design new crystals with specific physical and chemical properties (Lam & Mak, 2000). We have been interested in hydrogen-bonded systems formed by organic amines and carboxylic acids that generate molecular assemblies (Odabaşoğlu, Büyükgüngör & Lönnecke, 2003; Odabaşoğlu, Büyükgüngör, Turgut *et al.*, 2003; Büyükgüngör *et al.*, 2004; Büyükgüngör & Odabaşoğlu, 2002, 2003; Odabaşoğlu & Büyükgüngör, 2006*a,b*). The present work is part of a structural study of compounds of organic ammonium systems with hydrogen-bond donors and we report here the structure of the title compound, (I) (Fig. 1).



In (I), the 2-amino-6-methylpyridinium ions are linked to the 2-formylbenzoate ions through $\text{N}-\text{H} \cdots \text{O}$ hydrogen bonds and generate $[\text{R}_2^2(8)\text{R}_4^2(8)\text{R}_2^2(8)]$ motifs (Fig. 2 and Table 1). These motifs are connected by three $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds involving two water O atoms.

Experimental

The title compound was prepared by mixing 2-amino-6-methylpyridine and 2-formylbenzoic acid in a 1:1 molar ratio in 50 ml of

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water at room temperature. Crystals of (I) were obtained by slow evaporation of the solvent (m.p. 319–321 K).

Crystal data

$C_6H_9N_2^+ \cdot C_8H_5O_3^- \cdot H_2O$ $Z = 8$
 $M_r = 276.29$ $D_x = 1.341 \text{ Mg m}^{-3}$
 Monoclinic, $C2/c$ Mo $K\alpha$ radiation
 $a = 34.171 (3) \text{ \AA}$ $\mu = 0.10 \text{ mm}^{-1}$
 $b = 4.9220 (3) \text{ \AA}$ $T = 296 \text{ K}$
 $c = 19.4423 (17) \text{ \AA}$ Prism, colourless
 $\beta = 123.172 (6)^\circ$ $0.71 \times 0.38 \times 0.12 \text{ mm}$
 $V = 2737.1 (4) \text{ \AA}^3$

Data collection

Stoe IPDS2 diffractometer 14999 measured reflections
 ω scan 2400 independent reflections
 Absorption correction: integration 1794 reflections with $I > 2\sigma(I)$
 (*X-RED32*; Stoe & Cie, 2002) $R_{\text{int}} = 0.084$
 $T_{\text{min}} = 0.949$, $T_{\text{max}} = 0.991$ $\theta_{\text{max}} = 25.1^\circ$

Refinement

Refinement on F^2 $w = 1/[\sigma^2(F_o^2) + (0.0679P)^2 + 0.2766P]$
 $R[F^2 > 2\sigma(F^2)] = 0.041$ where $P = (F_o^2 + 2F_c^2)/3$
 $wR(F^2) = 0.117$ $(\Delta/\sigma)_{\text{max}} = 0.001$
 $S = 1.02$ $\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$
 2400 reflections $\Delta\rho_{\text{min}} = -0.18 \text{ e \AA}^{-3}$
 199 parameters Extinction correction: *SHELXL97*
 H atoms treated by a mixture of independent and constrained refinement Extinction coefficient: 0.0055 (9)

Table 1

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$N2-H2A \cdots O1^i$	0.87 (2)	2.10 (2)	2.939 (2)	163 (2)
$N2-H2B \cdots O1^{ii}$	0.92 (3)	2.06 (3)	2.980 (2)	171 (2)
$O4-H4A \cdots O1$	0.82 (2)	2.10 (2)	2.914 (2)	171 (3)
$O4-H4B \cdots O4^{iii}$	0.83 (2)	2.03 (2)	2.8681 (17)	179 (3)
$N1-H1 \cdots O2^{ii}$	0.86	1.81	2.6683 (19)	174

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

The amine and water H atoms were located in a difference Fourier map and refined freely with isotropic displacement parameters. All other H atoms were refined using the riding-model approximation, with $C-H = 0.93 \text{ \AA}$ for aromatic H atoms, $N-H = 0.86 \text{ \AA}$ for ring N atoms, and $C-H = 0.96 \text{ \AA}$ for methyl H atoms [$U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{parent atom})$ for all riding atoms].

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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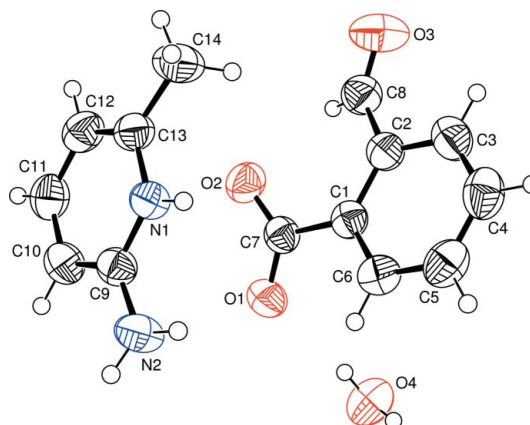


Figure 1 A view of (I), with the atomic numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

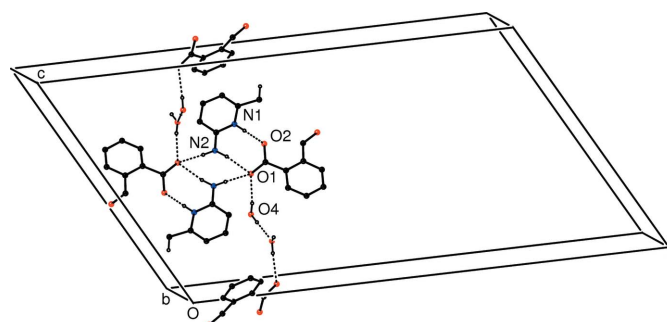


Figure 2 A partial packing diagram of (I), showing the hydrogen-bonding scheme with dashed lines. H atoms not involved in hydrogen bonding have been omitted.

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