

## Pyridinium 5-carboxypyrazine-2-carboxylate

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In the crystal structure of the title compound,  $C_5H_6N^{+} \cdot C_6H_3N_2O_4^{-}$ , the 5-carboxypyrazine-2-carboxylate (pdc) monoanion lies entirely on a mirror plane. The N and C atoms of the cation, together with their attached H atoms, lie on the same mirror plane. A supramolecular network is assembled between the pdc anions and pyridinium cations *via*  $N-H \cdots O$ ,  $O-H \cdots O$  and  $C-H \cdots O$  hydrogen bonding.

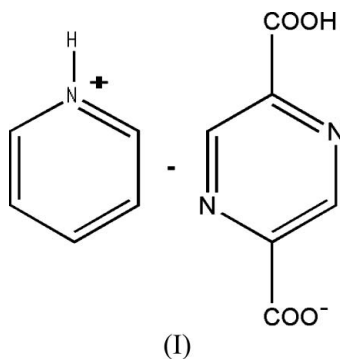
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## Key indicators

Single-crystal X-ray study  
 $T = 294$  K  
Mean  $\sigma(C-C) = 0.003$  Å  
 $R$  factor = 0.036  
 $wR$  factor = 0.109  
Data-to-parameter ratio = 11.0For details of how these key indicators were  
automatically derived from the article, see  
<http://journals.iucr.org/e>.

## Comment

By establishing appropriate connections between molecular and supramolecular structures on the basis of intermolecular interactions, crystal engineering is attracting more and more attention for its potential applications in materials science. Here, we report the crystal structure of the title compound, (I).



The crystal structure of (I) consists of 5-carboxypyrazine-2-carboxylate (pdc) monoanions and pyridinium anions (Fig. 1). The pdc is located entirely on a mirror plane. The C—O bond distances in the deprotonated carboxyl group are significantly different from those in the other (Table 1). In the pyridinium cation, atoms N3 and C9 and their attached H atoms also lie on a mirror plane.

Classical  $O-H \cdots O$ ,  $N-H \cdots O$  and weak  $C-H \cdots O$  hydrogen bonds occur in the crystal structure (Table 2), linking the cations and anions to form a supramolecular structure, as shown in Fig. 2.

## Experimental

A mixture of  $AgNO_3$  (0.0154 g, 0.09 mmol) and pyridine (30 ml) was stirred for some time, then Hpdc (0.015 g, 0.09 mmol) and dimethylsulfoxide (4 ml) were added and the mixture stirred for 1 h at room temperature. The mixture was filtered and single crystals of (I) were obtained from the filtrate after a month.

## Crystal data

$C_5H_6N^+ \cdot C_6H_3N_2O_4^-$   
 $M_r = 247.21$   
 Monoclinic,  $P2_1/m$   
 $a = 9.237(2) \text{ \AA}$   
 $b = 6.7553(18) \text{ \AA}$   
 $c = 9.529(3) \text{ \AA}$   
 $\beta = 115.905(4)^\circ$   
 $V = 534.9(2) \text{ \AA}^3$

$Z = 2$   
 $D_x = 1.535 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.12 \text{ mm}^{-1}$   
 $T = 294(2) \text{ K}$   
 Block, colourless  
 $0.28 \times 0.24 \times 0.20 \text{ mm}$

## Data collection

Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: none  
 3034 measured reflections

1195 independent reflections  
 943 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.019$   
 $\theta_{max} = 26.4^\circ$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.036$   
 $wR(F^2) = 0.109$   
 $S = 1.08$   
 1195 reflections  
 109 parameters  
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0544P)^2 + 0.1076P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.22 \text{ e \AA}^{-3}$   
 $\Delta\rho_{min} = -0.17 \text{ e \AA}^{-3}$   
 Extinction correction: *SHELXL97*  
 Extinction coefficient: 0.046 (8)

Table 1

Selected bond lengths (Å).

O1—C1	1.205 (2)	O3—C6	1.241 (2)
O2—C1	1.301 (2)	O4—C6	1.255 (2)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
$O2-H2 \cdots O4^i$	0.863 (10)	1.642 (11)	2.4964 (19)	170 (2)
$N3-H3A \cdots O3^i$	0.94 (3)	1.70 (3)	2.635 (2)	170 (2)
$C9-H9 \cdots O1^{ii}$	0.93	2.42	3.338 (2)	171

Symmetry codes: (i)  $x, y, z - 1$ ; (ii)  $x - 1, y, z$ .

H atoms bonded to N and O atoms were located in a difference Fourier map. Atom H3A was refined isotropically and atom H2 was refined with  $U_{iso}(H) = 1.2U_{eq}(O)$ . Aromatic H atoms were placed in calculated positions, with  $C-H = 0.93 \text{ \AA}$ , and refined in riding mode, with  $U_{iso}(H) = 1.2U_{eq}(C)$ .

Data collection: *SMART* (Bruker, 2003); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997a); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997a); molecular graphics:

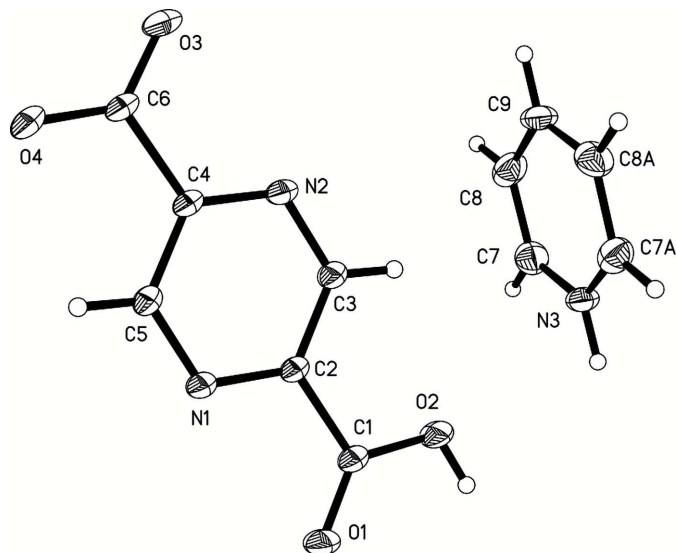


Figure 1

The structure of the ions of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms). [Symmetry code: (A)  $x, -y + \frac{1}{2}, z$ .]

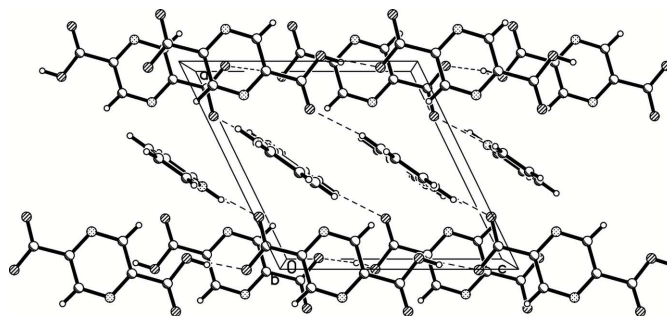


Figure 2

A view of the packing of (I). Dashed lines indicate hydrogen bonds.

*SHELXTL* (Sheldrick, 1997b); software used to prepare material for publication: *SHELXTL*.

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## References

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