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1-Carboxymethylpyridinium-2-carboxylate

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.055
wR factor = 0.158
Data-to-parameter ratio = 14.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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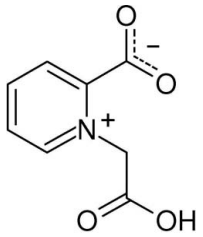
The title compound, $C_8H_7NO_4$, crystallizes with two independent molecules in the asymmetric unit, displaying different conformations. The molecules are linked into chains *via* O—H···O hydrogen bonds, and there are C—H···O interactions between chains.

Comment

By virtue of their overall neutral charge and naked carboxyl group, betaine and its derivatives can easily coordinate to metal atoms and can be used to prepare soluble metal complexes. To study the structure and the coordinated ability of this sort of compound, we synthesized and obtained crystals of the title organic complex, (I).

Compound (I) crystallizes with two independent molecules in the asymmetric unit, displaying different conformations (Fig. 1). Specifically, the dihedral angles between the plane of the pyridine ring and the plane of the deprotonated carboxylate group are 26.8 (1) and 32.1 (1)° in the two molecules, and the torsion angles C1—N1—C6—C7 and C9—N2—C14—C15 are 88.5 (1) and 68.6 (1)°, respectively.



(I)

The molecules are linked into chains *via* O—H···O hydrogen bonds (Table 1) and there are C—H···O interactions between chains.

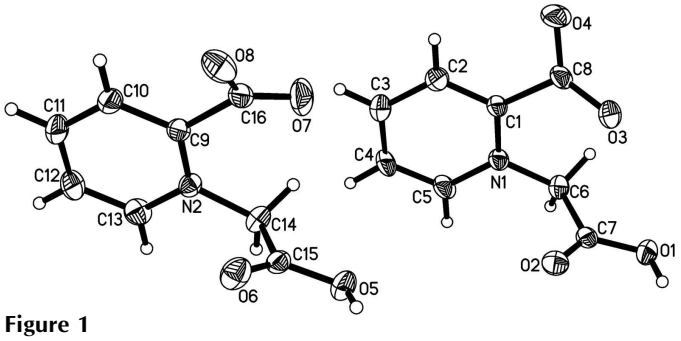


Figure 1
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are represented as spheres of arbitrary radius.

Experimental

Compound (I) was prepared by diffusion of HCl (7% concentration in water) into an aqueous solution (5 ml) of the sodium salt of 1-carboxymethyl-2-pyridinecarboxylic acid (0.204 g, 1 mmol) at room temperature. Single crystals of (I) were obtained after 3 d.

Crystal data

$C_8H_7NO_4$
M_r = 181.15
Monoclinic, $P2_1/n$
a = 7.9459 (12) Å
b = 11.5115 (18) Å
c = 17.826 (5) Å
β = 95.671 (17)°
V = 1622.5 (6) Å^3
Z = 8
D_x = 1.483 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.12 mm^{-1}
T = 293 (2) K
Block, colourless
0.25 × 0.23 × 0.20 mm

Data collection

Siemens $P4$ diffractometer
ω scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.970, T_{max} = 0.976
4683 measured reflections
3516 independent reflections
2248 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 27.0°
3 standard reflections
every 120 reflections
intensity decay: 8%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.158
S = 0.99
3516 reflections
237 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2 + 0.3152P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O8^{i}	0.82	1.76	2.540 (3)	160
O5—H5A···O4^{i}	0.82	1.69	2.499 (3)	168

Symmetry code: (i) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$.

All H atoms were placed in calculated positions and allowed to ride on their respective parent atoms, with C—H = 0.93–0.97 Å and O—H = 0.82 Å, and U_{iso}(H) = 1.2U_{eq}(C,O).

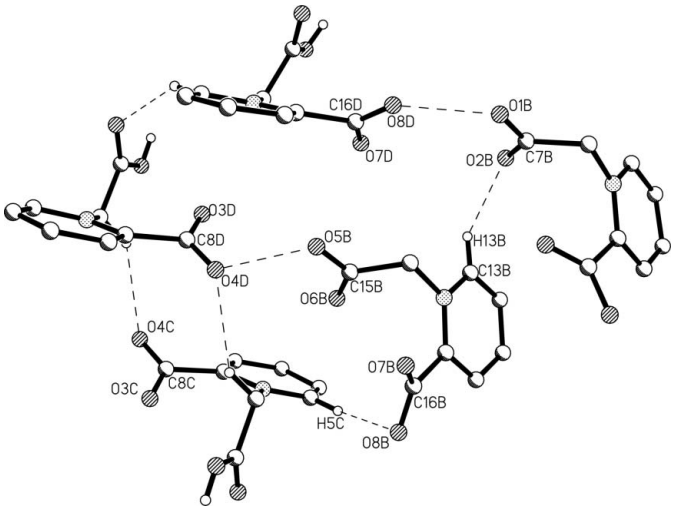


Figure 2
The extended structure of (I), formed through hydrogen-bonding interactions (dashed lines). H atoms not involved in hydrogen bonding have been omitted for clarity. [Symmetry code: (B) $1+x, y, z$; (C) $-x, 1-y, 1-z$; (D) $1-x, 1-y, 1-z$.]

Data collection: *XSCANS* (Siemens, 1994); cell refinement: *XSCANS*; data reduction: *XSCANS*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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1-Carboxymethylpyridinium-2-carboxylate. Corrigendum

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The authors listed in the original report by Song, Li & Song [*Acta Cryst.* (2006), E**62**, o4656–o4657] are incorrect. The correct author of the paper is given here and is the sole author of the paper.