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Key indicators

Single-crystal X-ray study

$T = 115\text{ K}$

Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$

R factor = 0.028

wR factor = 0.068

Data-to-parameter ratio = 41.0

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

4-Amino-(1-ethoxycarbonylmethyl)pyridinium iodide

The crystal structure of the title compound, $\text{C}_9\text{H}_{13}\text{N}_2\text{O}_2^+\cdot\text{I}^-$, consists of pyridinium cations and iodide anions stabilized by intermolecular $\text{N}-\text{H}\cdots\text{I}$ hydrogen bonds, forming one-dimensional chains along $[010]$.

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Comment

Pyridinium derivatives often possess antibacterial and antifungal activities (Seethalakshmi *et al.*, 2006, and references therein). In continuation of our study of pyridinium derivatives, the crystal structure analysis of the title compound, (I), has been undertaken.

The structure of the asymmetric unit of (I), consisting of a pyridinium cation and an iodide anion, is shown in Fig. 1. The bond lengths and angles within the pyridinium ring are normal and comparable with those reported for related structures (Seethalakshmi *et al.*, 2006; Sundar *et al.*, 2004*a,b*, 2005; Sundar *et al.*, 2006, 2006*a,b*). The $\text{N1}-\text{C6}-\text{C7}-\text{O1}$, $\text{C6}-\text{C7}-\text{O1}-\text{C8}$ and $\text{C7}-\text{O1}-\text{C8}-\text{C9}$ torsion angles in (I) (Table 1) indicate that the ethoxycarbonylmethyl group is in an extended conformation. Atoms $\text{N1}/\text{C6}/\text{C7}/\text{O1}/\text{C8}/\text{C9}$ form an approximate plane with a maximum deviation of $0.193(2)\text{ \AA}$ for C6; the dihedral angle between this plane and the pyridinium ring is $66.1(1)^\circ$.

In the crystal structure of (I), neighbouring pyridinium cations are interconnected by iodide anions through intermolecular $\text{N}-\text{H}\cdots\text{I}$ hydrogen bonds (Fig. 2 and Table 2), leading to a one-dimensional chain along $[010]$. In addition to these interactions, a weak intermolecular $\text{C}-\text{H}\cdots\text{I}$ inter-

Figure 1

The asymmetric unit of (I), showing displacement ellipsoids drawn at the 50% probability level. H atoms are represented by circles of arbitrary radii.

Figure 2

Part of the crystal structure of (I), viewed along the *a* axis. The intermolecular non-bonded $N \cdots I$ distances of the $N-H \cdots I$ hydrogen bonds are indicated by dashed lines. H atoms have been omitted.

action also is observed, involving the H atom bonded to C1 and I1 [$C1 \cdots I1 = 3.773(2) \text{ \AA}$, $H1 \cdots I1 = 2.92 \text{ \AA}$ and $C1-H1 \cdots I1 = 150^\circ$].

Experimental

A solution of 4-aminopyridine (1 mol, 25 ml) and ethyl α -iodoacetate (1 mol, 25 ml) in acetone was stirred at room temperature (303 K) for 1–2 h. The solid that separated was filtered, washed with dry acetone and dried in vacuum to give the stable salt, (I), which recrystallized from an aqueous ethanol (80% *v/v*) solution (m.p. 449–451 K).

Crystal data

$C_9H_{13}N_2O_2^+ \cdot I^-$
 $M_r = 308.11$
 Orthorhombic, *Pbcn*
 $a = 12.5402(15) \text{ \AA}$
 $b = 9.8173(10) \text{ \AA}$
 $c = 19.135(2) \text{ \AA}$
 $V = 2355.7(4) \text{ \AA}^3$

$Z = 8$
 $D_x = 1.738 \text{ Mg m}^{-3}$
 Mo $K\alpha$ radiation
 $\mu = 2.70 \text{ mm}^{-1}$
 $T = 115(2) \text{ K}$
 Fragment, colorless
 $0.25 \times 0.22 \times 0.20 \text{ mm}$

Data collection

Bruker–Nonius KappaCCD
 diffractometer
 ω scans with κ offsets
 Absorption correction: multi-scan
 (SCALEPACK; Otwinowski &
 Minor, 1997)
 $T_{\min} = 0.524$, $T_{\max} = 0.583$

36052 measured reflections
 5535 independent reflections
 4300 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.021$
 $\theta_{\max} = 36.4^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.068$
 $S = 1.06$
 5535 reflections
 135 parameters
 H atoms treated by a mixture of
 independent and constrained
 refinement

$w = 1/[\sigma^2(F_o^2) + (0.0272P)^2 + 1.6703P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 1.37 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.96 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL97
 Extinction coefficient: 0.00249 (13)

Table 1

Selected torsion angles ($^\circ$).

C8–O1–C7–C6	167.70 (14)	C7–O1–C8–C9	−177.72 (16)
N1–C6–C7–O1	161.57 (14)		

Table 2

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

$D-H \cdots A$	$D-H$	$H \cdots A$	$D \cdots A$	$D-H \cdots A$
N2–H21 $\cdots$ I1	0.85 (3)	2.79 (3)	3.6384 (17)	173 (2)
N2–H22 $\cdots$ I1 ⁱ	0.79 (3)	2.91 (2)	3.6527 (17)	159 (2)

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

The amino H atoms were located in a difference Fourier map and refined with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{N})$. The methyl H atoms were constrained to an ideal geometry ($C-H = 0.98 \text{ \AA}$), with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$, but were allowed to rotate freely about the $C-C$ bond. The remaining H atoms were placed in geometrically idealized positions ($C-H = 0.95\text{--}0.99 \text{ \AA}$) and were constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. The highest residual density peak is $0.68 \text{ \AA}$ from I1 and the deepest hole is $0.67 \text{ \AA}$ from I1.

Data collection: *COLLECT* (Nonius, 2000); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (version 1.07; Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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