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Quinolinium fumarate

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Key indicators

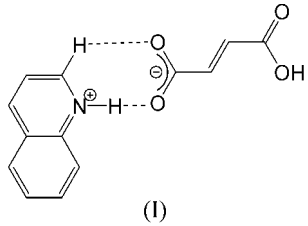
Single-crystal X-ray study
T = 140 K
Mean σ(C–C) = 0.002 Å
R factor = 0.034
wR factor = 0.085
Data-to-parameter ratio = 14.3

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

In the title complex, $C_9H_8N^+\cdot C_4H_3O_4^-$, fumarate anions are linked by O—H···O hydrogen bonds, forming infinite supramolecular chains along the c axis. Quinolinium cations are attached to the anionic chains *via* N—H···O and C—H···O interactions. The crystal structure determination confirms the protonation of the quinoline N atom and deprotonation of one of the carboxylic acid groups of fumaric acid.

Comment

Fumaric acid is an organic dicarboxylic acid which crystallizes in two polymorphic forms: one in the monoclinic space group $P2_1/c$ (Brown, 1966) and the other in the triclinic space group $P\overline{1}$ (Bednowitz & Post, 1966). In both crystal structures, acid molecules are linked by carboxylic acid $R_2^2(8)$ hydrogen-bond pairs, forming one-dimensional supramolecular tapes. Fumaric acid is of interest since it is known to form supramolecular assemblies with N-aromatic complexes (Batchelor *et al.*, 2000). As part of our analysis of supramolecular architectures, the structure of the title complex, (I), was determined at 140 K.



(I)

(I) consists of a 1:1 complex of fumarate anions and quinolinium cations. The asymmetric unit and atomic numbering scheme are shown in Fig. 1. Zigzag supramolecular acid chains are formed along the c axis *via* O1—H01···O3 hydrogen bonds (Table 2). In addition, quinolinium cations are linked to the acid chains (Fig. 2) by N1—H02···O4 hydrogen bonds and C9—H9···O3 interactions. Proton transfer is observed between the carboxylic acid group and the quinoline N atom (Table 1). Quinolinium cations form infinite stacks along the b axis, the distance between adjacent molecules within a stack being *ca* 3.5 Å.

Experimental

Fumaric acid and quinoline were obtained from Aldrich without further purification. 46 mg of the acid and 52 mg of the base were mixed and dissolved in a mixture of 9 ml of ethyl acetate and 10 drops of methanol. Crystals of (I) were obtained by slow evaporation at room temperature.

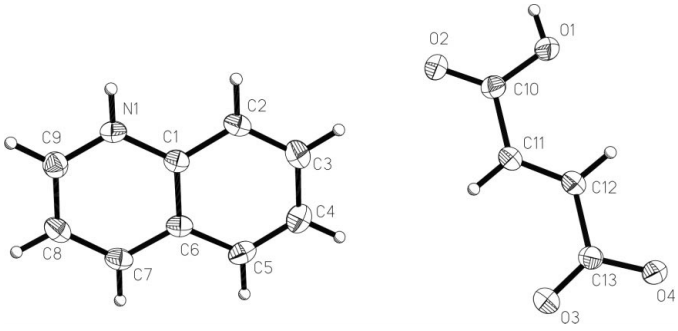


Figure 1
The molecular unit of (I), showing displacement ellipsoids at the 50% probability level (*XP*; Sheldrick, 1993).

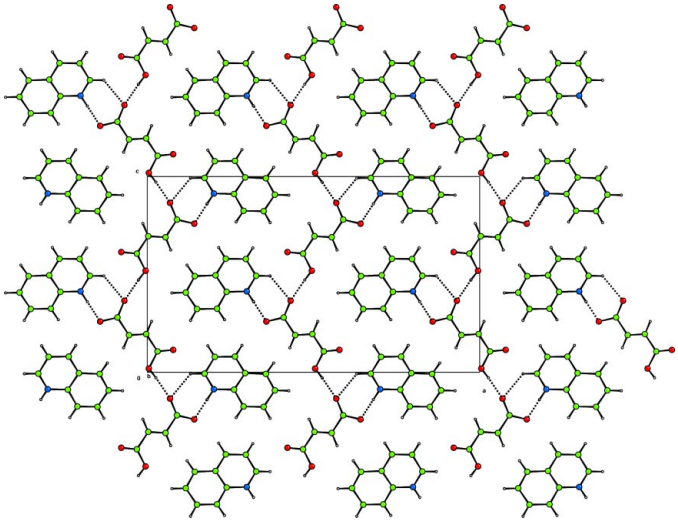


Figure 2
Projection on to (010), showing the zigzag supramolecular tapes formed by O—H···O hydrogen bonds and proton transfer between the carboxylic acid and the aromatic N atom (*CAMERON*; Watkin *et al.*, 1996).

Crystal data

$C_9H_8N^+\cdot C_4H_3O_4^-$
M_r = 245.23
Orthorhombic, $Pca2_1$
a = 22.5838 (5) Å
b = 3.7273 (1) Å
c = 13.2912 (5) Å
V = 1118.81 (6) Å^3
Z = 4
D_x = 1.456 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9880 reflections
θ = 1.8–27.5°
μ = 0.11 mm^{-1}
T = 140 (2) K
Block, colourless
0.23 × 0.23 × 0.16 mm

Data collection

Nonius KappaCCD diffractometer
Thin-slice ω and φ scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.877, T_{max} = 0.985
9868 measured reflections
2329 independent reflections
2118 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
θ_{max} = 27.5°
$h = -23 \rightarrow 29$
$k = -4 \rightarrow 3$
$l = -17 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.085
S = 1.08
2325 reflections
163 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.0496P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

Table 1
Selected geometric parameters (Å).

O2—C10	1.207 (2)	O3—C13	1.233 (2)
O4—C13	1.282 (2)	O1—C10	1.330 (2)

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H02···O4^{i}	0.88	1.67	2.553 (2)	179
C9—H9···O3^{i}	0.95	2.79	3.348 (2)	119
O1—H01···O3^{ii}	0.84	1.83	2.667 (2)	177
C3—H3···O2	0.95	2.35	3.284 (2)	168

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

All H atoms bonded to C atoms were placed geometrically and refined using a riding model, with U_{iso} for each H atom taken as $1.2U_{eq}$ of the carrier atom. Atoms H01 and H02 were located from a difference Fourier map and refined using a riding model. The absolute structure was not determined. Friedel opposites were merged prior to merging of data in $Pca2_1$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *HKL DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* (Sheldrick, 1993); software used to prepare material for publication: *SHELXL*97.

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