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Acridinium isophthalate

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The crystal structure of the title complex, $C_{13}H_{10}N^+\cdot C_8H_5O_4^-$, confirmed the full proton transfer, *i.e.* protonation of the acridine N atom and deprotonation of one of the carboxylic acid groups, in the isophthalic (1,3-benzenedicarboxylic) acid. In the title complex, isophthalate anions are linked *via* strong O—H···O bonds and weak C—H···O bonds into infinite chains along the *a* axis of the crystal. The acridinium cations are attached to the anionic chains *via* strong hydrogen bonds involving the carboxylate groups of the isophthalate anion and the NH group of the acridinium cation.

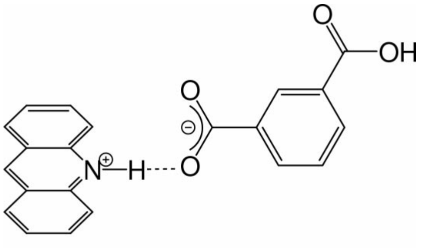
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.004 Å
R factor = 0.045
wR factor = 0.120
Data-to-parameter ratio = 12.0

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

Comment

Isophthalic acid is an organic dicarboxylic acid which crystallizes in space group $P2_1/c$, and forms supramolecular acid chains in its solid-state structure (Derissen, 1974). It is one of the organic acids that we are interested in for our research into the molecular self-assembly of carboxylic acids with N-aromatic complexes. As part of our analysis of the molecular interactions, the structure of the title complex, (I), was determined.



(I)

In (I), the cations and anions form a 1:1 cocrystal. The asymmetric unit and atomic numbering scheme of (I) is shown in Fig. 1. Supramolecular acid chains are formed along the *a* axis *via* strong O3—H101···O2 and weak C19—H19···O4 hydrogen bonds (Table 2). In addition, acridinium cations are joined to the acid chains (Fig. 2) by N1—H1···O1 hydrogen bonds (Table 2). Proton transfer occurs between the carboxylic acid group and the acridine N atom so that the aromatic N atom is positively charged while the corresponding carboxylic acid group is negatively charged (Table 1). Acridinium cations form infinite stacks along the *a* axis, the distance between the planes of adjacent acridinium cations being *ca* 3.5 Å.

Experimental

Acridine and isophthalic acid were obtained from Aldrich. 33 mg of the acid and 36 mg of the base were used to dissolve into 15 ml of

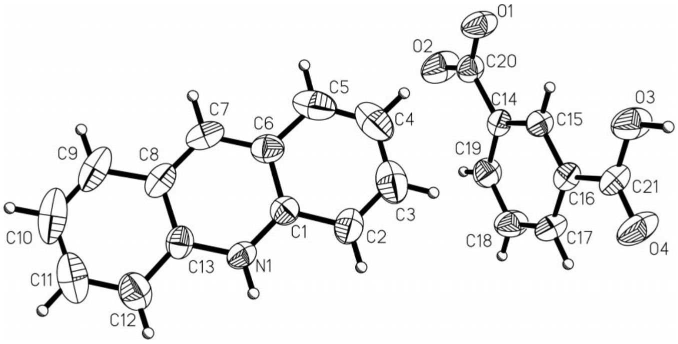


Figure 1
The acridinium cation and isophthalate anion in the crystal structure of (I). Displacement ellipsoids are drawn at the 50% probability level (*XP*; Sheldrick, 1993).

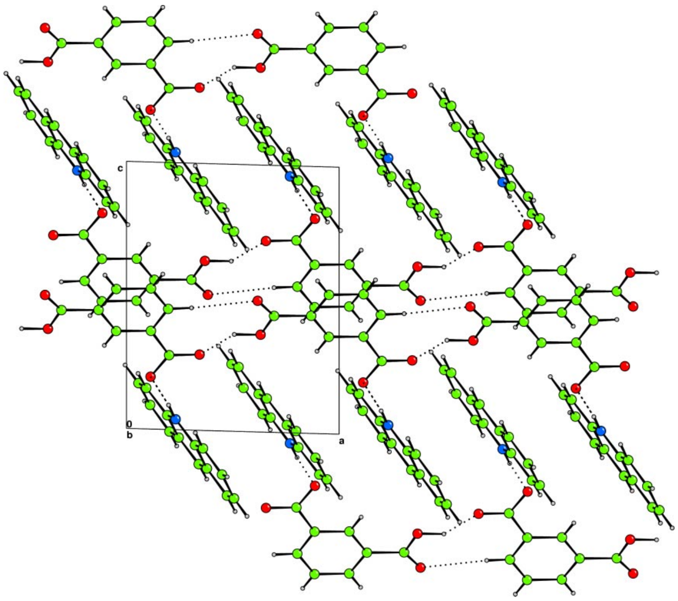


Figure 2
Projection of the molecular packing of (I) on to the (010) plane showing isophthalate chains and acridinium stacks (*CAMERON*; Watkin *et al.*, 1996).

ethanol. Crystals of (I) were obtained by slow evaporation of the ethanol solution at room temperature.

Crystal data

$C_{13}H_{10}N^+ \cdot C_8H_5O_4^-$
$M_r = 345.34$
Triclinic, $P\bar{1}$
$a = 8.5196$ (9) Å
$b = 9.1440$ (10) Å
$c = 11.386$ (4) Å
$\alpha = 69.41$ (2)°
$\beta = 89.440$ (10)°
$\gamma = 84.220$ (10)°
$V = 825.8$ (3) Å^3
$Z = 2$
$D_x = 1.389$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 25 reflections
$\theta = 8.0$–15.0°
$\mu = 0.10$ mm^{-1}
$T = 295$ (2) K
Block, yellow
0.50 × 0.25 × 0.15 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
3032 measured reflections
2874 independent reflections
2054 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\rm max} = 24.9°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = 0 \rightarrow 13$
3 standard reflections every 200 reflections intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.120$
$S = 1.11$
2874 reflections
239 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0389P)^2 + 0.2511P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.16$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.27$ e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—C20	1.272 (2)	O3—C21	1.316 (3)
O2—C20	1.219 (2)	O4—C21	1.205 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H101···O2$^{\rm i}$	1.06 (3)	1.61 (3)	2.562 (2)	147 (3)
N1—H1···O1$^{\rm ii}$	0.86	1.70	2.553 (2)	173
C19—H19···O4$^{\rm iii}$	0.93	2.66	3.582 (3)	174

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

The H101 atom on the carboxylic acid group was located from the difference Fourier map and refined without restraint. All other H atoms were placed geometrically and allowed to ride on their parent atom during subsequent refinement, with an isotropic displacement parameter fixed at 1.2 times the $U_{\rm eq}$ value of the corresponding C or N atom.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1988); cell refinement: *CAD*-4 *Software*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1995); 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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