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3-Hydroxypyridinium 1-carboxybenzene-3-carboxylate

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The asymmetric unit of the title organic salt, $C_5H_6NO^+\cdot C_8H_5O_4^-$, comprises a 3-hydroxypyridinium cation and one singly deprotonated 1,3-benzenedicarboxylic acid anion. The cations and anions are linked by N—H···O and O—H···O hydrogen bonds to form a two-dimensional array.

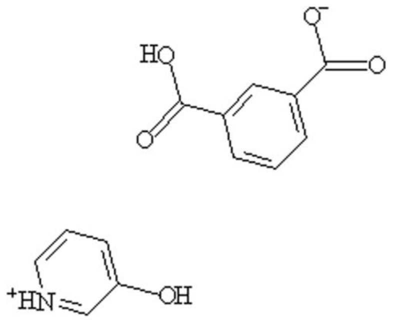
Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.003 Å
R factor = 0.042
wR factor = 0.123
Data-to-parameter ratio = 12.4

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

Comment

One of the goals of organic crystal engineering is the rational design and preparation of molecular architectures with robust structures and functions (Brammer, 2004; Steiner, 2002). Up to now, aromatic polycarboxylic acids have been used extensively in the synthesis of coordination polymers (Wen *et al.*, 2005) and the generation of hydrogen-bonded arrays of organic cocrystals (Bowers *et al.*, 2005). Bifunctional 3-hydroxypyridine (3-HP) has one hydrogen-bond-accepting heterocyclic N atom and a hydrogen-bond-donating hydroxy group, which is not only capable of binding to metal centers (Kawata *et al.*, 1997; Castillo *et al.*, 2000; Gao *et al.*, 2004), but can also form regular hydrogen bonds by functioning as both hydrogen-bond donor and acceptor (Breeze & Wang, 1993). Our interest in this area has focused upon the synthesis of metal complexes with 1,3-benzenedicarboxylate (1,3-BDC) and 3-HP. Compound (I) was isolated during the attempted synthesis of a Cu complex. Compound (I) comprises a 3-hydroxypyridinium cation and a singly deprotonated 1,3-benzenedicarboxylic acid anion (Fig. 1). A two-dimensional supramolecular structure is formed *via* intermolecular hydrogen bonds between the carboxyl atoms (O2, O3 and O4) of 1,3-BDC and the hydroxy group and N atom of 3-HP (Table 1 and Fig. 2).



(I)

Experimental

Compound (I) was isolated from the following attempted synthesis using hydrothermal methods. A mixture of an aqueous solution of

1,3-benzenedicarboxylic acid (0.5 mmol) that had been neutralized with sodium hydroxide (1 mmol), 3-hydroxypyridine (1 mmol), $Cu(ClO_4)_2 \cdot 6H_2O$ (0.5 mmol) and water (15.0 ml) was placed in a 23 ml Teflon-lined stainless steel reactor. The solution was heated at 413 K for 3 d. After reaction, the vessel was cooled slowly to room temperature to give brown crystals. The crystals were collected, washed with distilled water and dried in air. Analysis calculated for $C_{13}H_{11}NO_5$: C 59.77, H 4.24, N 5.36%; found: C 60.17, H 4.25, N 5.38%.

Crystal data

$C_5H_6NO^+ \cdot C_8H_5O_4^-$
$M_r = 261.23$
Monoclinic, $P2_1/n$
$a = 10.2943$ (17) Å
$b = 10.9947$ (18) Å
$c = 10.4059$ (17) Å
$\beta = 99.963$ (2)°
$V = 1160.0$ (3) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.12$ mm^{-1}
$T = 291$ (2) K
0.26 × 0.15 × 0.09 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.971$, $T_{max} = 0.990$
8655 measured reflections
2160 independent reflections
1337 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.123$
$S = 1.03$
2160 reflections
174 parameters
H-atom parameters constrained
$\Delta\rho_{max} = 0.15$ 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
N1—H1···O3^{i}	0.86	1.79	2.649 (2)	177
O5—H5···O4^{ii}	0.82	1.81	2.619 (2)	169
O2—H2···O3^{iii}	0.82	1.88	2.670 (2)	161

Symmetry codes: (i) $x, y+1, z-1$; (ii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iii) $-x, -y, -z+1$.

All H atoms were included in the riding model approximation with O—H = 0.82 Å, N—H = 0.86 Å and C—H = 0.93 Å, and with $U_{iso}(H) = 1.2U_{eq}$(carrier) or $1.5U_{eq}$(carrier).

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2004); software used to prepare material for publication: *SHELXTL*.

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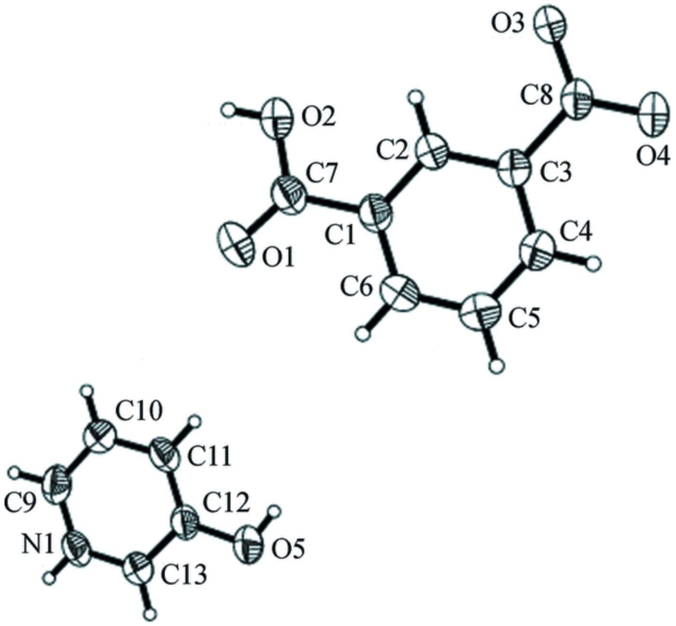

Figure 1
The molecular structures of the constituents of (I), showing the atom-numbering scheme and 50% proability displacement ellipsoids.

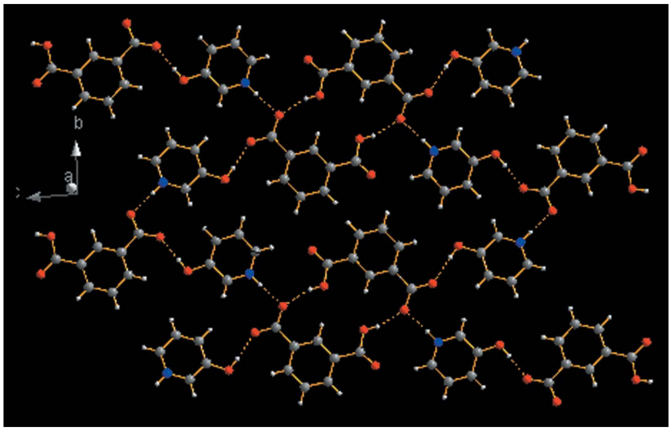

Figure 2
Part of the crystal structure of (I), showing the formation of a sheet built from N—H···O and O—H···O hydrogen bonds, shown as dashed lines.

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