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2,6-Dimethylpyridinium 2,4-dihydroxybenzoate 2,6-dimethylpyridine solvate

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The asymmetric unit of the title salt, $C_7H_{10}N^+\cdot C_7H_5O_4^-\cdot C_7H_9N$, consists of one 2,6-dimethylpyridinium cation, one 2,4-dihydroxybenzoate anion and one 2,6-dimethylpyridine solvent molecule, which form 1:1:1 associations by way of $N—H\cdots O$ and $O—H\cdots N$ hydrogen bonds. These entities then interact by way of $C—H\cdots\pi$ and $\pi–\pi$ interactions.

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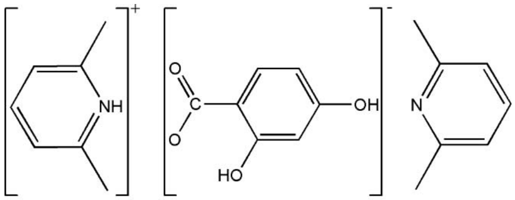
Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.152
Data-to-parameter ratio = 14.9

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

Comment

This work continues our previous synthetic and structural studies of supramolecular interactions in aromatic molecular salts and adducts (Wang & Wei, 2006).



(I)

The asymmetric unit of the title compound, (I), contains one 2,6-dimethylpyridinium cation, one 2,4-dihydroxybenzoate anion and one 2,6-dimethylpyridine solvent molecule (Fig. 1). The three components are linked together by a cation-to-anion $N—H\cdots O$ and an anion-to-solvent $O—H\cdots N$ hydrogen bond (Table 1). An intramolecular $O—H\cdots O$ interaction is also present in the anion.

The N2/C15–C19 ring makes weak $\pi–\pi$ interactions with its symmetry-related neighbours at $(x, \frac{1}{2} - y, -\frac{1}{2} + z)$ and $(x, \frac{1}{2} - y, \frac{1}{2} + z)$ positions with o-centroid distances of 3.9060 (12) Å in both cases. Similar weak $\pi–\pi$ interactions are observed between the N1/C8–C12 ring of the solvent molecule and its symmetry-related rings at $(x, \frac{3}{2} - y, -\frac{1}{2} + z)$ and $(x, \frac{3}{2} - y, \frac{1}{2} + z)$ with centroid separations of 3.9480 (13) Å.

Finally, $C—H\cdots\pi$ interactions occur in the crystal structure of (I). The 2,6-dimethylpyridine solvent molecule interacts with the C1–C6 ring (centroid C_g) of a 2,4-dihydroxybenzoate anion at the symmetry position $(1 - x, 1 - y, 2 - z)$ [$H\cdots C_g$ = 2.64 Å]. In addition, a 2,6-dimethylpyridinium cation interacts with another C1–C6 ring at the symmetry position $(-x, -\frac{1}{2} + y, \frac{3}{2} - z)$ with $H\cdots C_g$ = 2.84 Å. Together, these interactions result in a three-dimensional supramolecular network (Fig. 2).

Experimental

2,4-Dihydroxybenzoic acid (2.0 mmol, 0.31 g) was dissolved in 15 ml 2,6-dimethylpyridine. The mixture was stirred for 20 minutes at

343 K. The solution was filtered, and the filtrate was kept at room temperature. Colorless crystals of (I) were obtained from the filtrate after six days.

Crystal data

$C_7H_{10}N^+\cdot C_7H_5O_4^-\cdot C_7H_9N$
$M_r = 368.42$
Monoclinic, $P2_1/c$
$a = 16.0942$ (14) Å
$b = 15.7871$ (14) Å
$c = 7.7950$ (7) Å
$\beta = 97.217$ (1)°
$V = 1964.9$ (3) Å^3
$Z = 4$
$D_x = 1.245$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 292$ (2) K
Block, colorless
0.35 × 0.30 × 0.30 mm

Data collection

Bruker SMART APEX CCD diffractometer
ω scans
Absorption correction: none
14075 measured reflections
3846 independent reflections
2658 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.033$
$\theta_{\rm max} = 26.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.152$
$S = 1.06$
3846 reflections
258 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0889P)^2 + 0.0787P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.16$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.18$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O2	0.847 (10)	1.747 (15)	2.538 (2)	154 (3)
O4—H4···N1	0.832 (10)	1.910 (12)	2.723 (2)	165 (3)
N2—H22···O1	0.886 (10)	1.699 (11)	2.581 (2)	173 (3)

The N- and O-bound H atom was located in a difference map and refined with bond-distance restraints of 0.89 (1) and 0.85 (1) Å, respectively. The C-bound H atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(aromatic C) or 1.5$U_{\rm eq}$(methyl C,O).

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

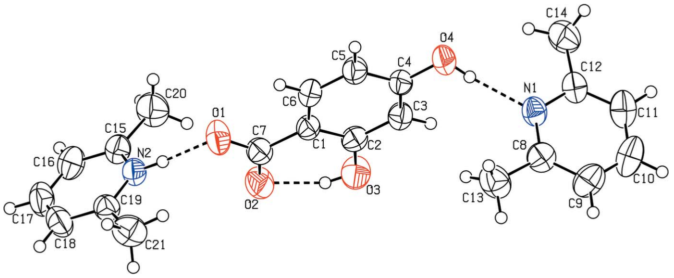


Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms). Hydrogen bonds are indicated by dashed lines.

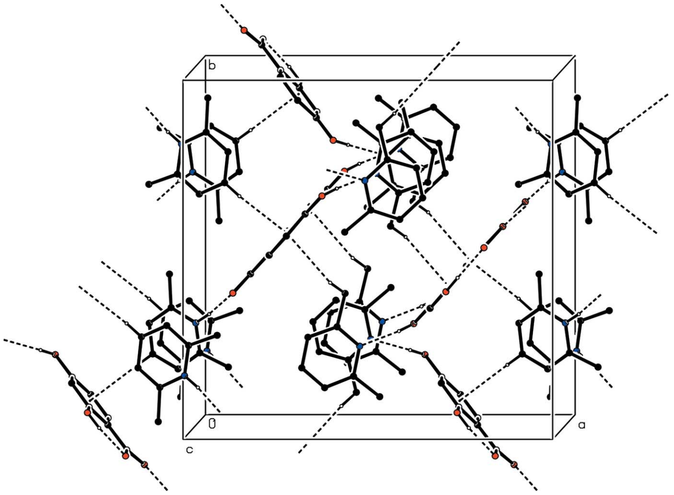


Figure 2
The packing digram of (I). Hydrogen bonds are shown as dashed lines. For clarity, H atoms not involved in hydrogen bonds are omitted.

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