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4,4′-Bipyridinium bis(2-carboxybenzenesulfonate) dihydrate

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The title compound, $C_{10}H_{10}N_2^{2+}\cdot 2C_7H_5O_5S_2^{-}\cdot 2H_2O$, consists of diprotonated 4,4′-bipyridinium cations, 2-sulfonatobenzoic acid anions and water molecules of crystallization, linked by N—H···O and O—H···O hydrogen bonds. The cation has crystallographic twofold rotation symmetry.

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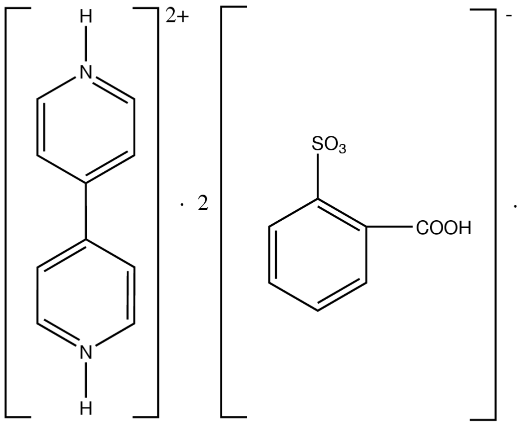
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.121
Data-to-parameter ratio = 13.5

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

Comment

4,4′-Bipyridine acts as a bridging ligand in the preparation of metal complexes (Tong *et al.*, 2000), as a host molecule in the formation of inclusion compounds (Lu *et al.*, 2001), and as a proton receptor in charge transfer complexes (Zhu, 2003). In this paper, we report the structure of the title compound, 4,4′-bipyridinium bis(2-carboxybenzenesulfonate) dihydrate, (I).



(I)

The title compound, (I), consists of diprotonated 4,4′-bipyridinium cations with crystallographic twofold rotation

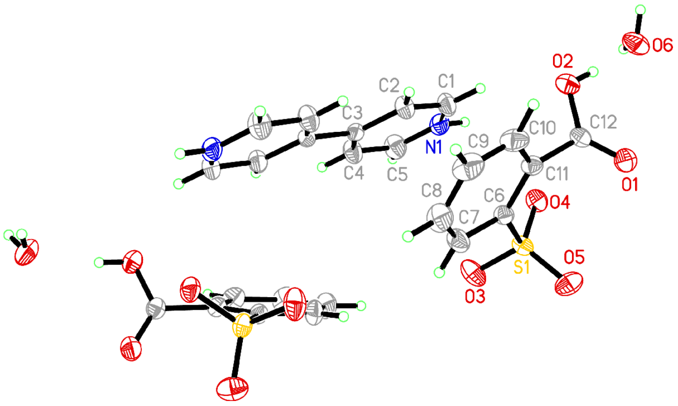


Figure 1
The structure of (I), with the atom numbering, showing displacement ellipsoids for non-H atoms at the 50% probability level (Johnson, 1976). H atoms are represented as small spheres.

symmetry, 2-carboxybenzenesulfonate anions and solvent water molecules (Fig. 1). The 4,4′-bipyridinium cations are linked to the the sulfonate and carboxy groups of the 2-carboxybenzenesulfonate anions through N—H⋯O hydrogen-bonding interactions (Table 1 and Fig. 2). The solvent water molecules form hydrogen bonds with both the carboxylic acid and sulfonate groups (Table 2).

Experimental

The title compound, (I), was isolated from the hydrothermal reaction of a mixture of bismuth nitrate pentahydrate (0.70 g, 2 mmol), 4,4′-bipyridine (0.32 g, 2 mmol), 5-nitroisophthalic acid (0.50 g, 2 mmol), 2,2′-dithiosalicylic acid (1.5 g, 4 mmol) and water (20 ml) in a 30 ml Teflon-lined stainless steel reactor. The solution was heated to 428 K for 4 d. The reaction system was then slowly cooled to room temperature, giving yellow crystals which were collected, washed with distilled water and dried in air. As shown by the results of the crystal structure determination, under these reaction conditions, the bismuth nitrate and 5-nitroisophthalic acid were not incorporated into the product and the 2,2′-dithiosalicylic acid decomposed to form 2-carboxybenzenesulfonate.

Crystal data

$C_{10}H_{10}N_2^{+}\cdot 2C_7H_5O_5S^{-}\cdot 2H_2O$
$M_r = 596.57$
Monoclinic, $C2/c$
$a = 13.9733\ (13)$ Å
$b = 12.2519\ (13)$ Å
$c = 15.0884\ (14)$ Å
$\beta = 94.558\ (2)^\circ$
$V = 2575.0\ (4)$ Å^3
$Z = 4$

$D_x = 1.539$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2537 reflections
$\theta = 2.8$–25.2°
$\mu = 0.28$ mm^{-1}
$T = 298\ (2)$ K
Block, yellow
0.44 × 0.39 × 0.38 mm

Data collection

Bruker SMART APEX area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2002)
$T_{\min} = 0.883$, $T_{\max} = 0.901$
7177 measured reflections

2537 independent reflections
2404 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.018$
$\theta_{\max} = 26.0^\circ$
$h = -17 \rightarrow 17$
$k = -14 \rightarrow 15$
$l = -10 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.121$
$S = 1.10$
2537 reflections
188 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0627P)^2 + 2.2842P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.48$ e Å^{-3}
$\Delta\rho_{\min} = -0.34$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—O5	1.4430 (17)	O1—C12	1.200 (3)
S1—O3	1.4499 (16)	O2—C12	1.317 (3)
S1—O4	1.4506 (14)	N1—C1	1.323 (3)
S1—C6	1.7794 (19)	N1—C5	1.324 (3)
O5—S1—O3	112.92 (11)	O2—C12—C11	111.37 (17)
O5—S1—O4	113.59 (10)	C1—N1—C5	122.20 (18)
O3—S1—O4	111.39 (10)	N1—C1—C2	120.3 (2)
O1—C12—O2	124.42 (19)	N1—C5—C4	119.9 (2)
O1—C12—C11	124.19 (19)		

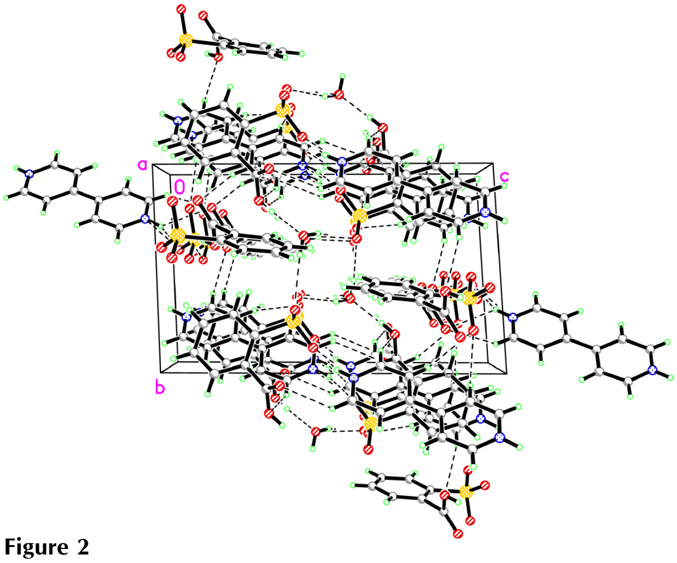


Figure 2
Perspective view of the molecular packing of (I), with hydrogen bonds shown as dashed lines.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O6—H6*B*⋯O3$^{\rm i}$	0.820 (10)	1.964 (13)	2.771 (3)	168 (3)
O6—H6*A*⋯O3$^{\rm ii}$	0.817 (10)	2.058 (14)	2.853 (2)	164 (3)
N1—H1N⋯O1$^{\rm ii}$	0.86	2.57	3.158 (3)	126
N1—H1N⋯O4$^{\rm ii}$	0.86	1.93	2.729 (2)	153
O2—H2*A*⋯O6	0.82	1.80	2.613 (2)	170

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

The water H atoms were refined subject to the restraint O—H = 0.82 (1) Å. The other H atoms were positioned geometrically and allowed to ride on their parent atoms at distances of 0.93 (C—H), 0.86 (N—H) and 0.82 Å ($O_{\rm COOH}$—H), with $U_{\rm iso} = 1.2U_{\rm eq}$(parent atom).

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL*(Bruker, 2000); software used to prepare material for publication: *SHELXL*97.

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