4,4′-Bipyridinium 1,5-naphthalenedisulfonate dihydrate

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Key indicators

Single-crystal X-ray study
$T = 298$ K
Mean σ(C–C) = 0.003 Å
R factor = 0.049
wR factor = 0.134
Data-to-parameter ratio = 14.6

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

The cation and anion of $C_{10}H_{10}N_2^{2+} \cdot C_{10}H_6O_6S_2^{2-} \cdot 2H_2O$ lie on different twofold rotation axes in the crystal structure. The cations, anions and water molecules are connected by hydrogen bonds into a three-dimensional network structure.

Comment

1,5-Naphthalenedisulfonic acid readily affords ammonium sulfonates with amines, and the crystallographically authenticated salts include, for example, diammonium 1,5-naphthalenedisulfonate (Sakwa & Wheeler, 2003). The sulfonate $-SO_3$ unit has a high propensity to form hydrogen bonds; in the present 4,4′-bipyridinium salt, (I), the compound crystallizes as a dihydrate (scheme and Fig. 1). The cations and anions interact through hydrogen bonds (Table 2) to furnish a three-dimensional network structure. The pyridinium H atom forms hydrogen bonds to the water and a sulfonate O atom (Fig. 2). The pyridinium H atom in the dihydrated 4-hydroxy-3-carboxybenzenesulfonate forms only one hydrogen bond to a sulfonate O atom [2.698 (3) Å] (Muthiah *et al.*, 2003).

(I)
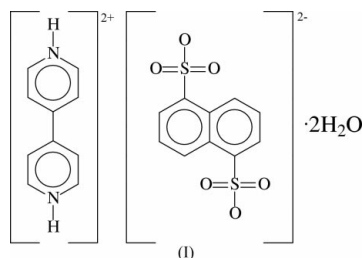
Experimental

Crystals of the compound separated from an aqueous solution of 4,4′-bipyridine (0.03 g, 0.2 mmol) and 1,5-naphthalenedisulfonic acid
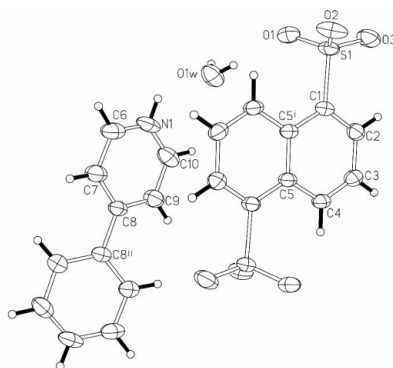

Figure 1
ORTEP (Johnson, 1976) plot of $[C_{10}H_{10}N_2][C_{10}H_6O_6S_2] \cdot 2H_2O$ with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. [Symmetry code (i) $1 - x, y, \frac{3}{2} - z$; (ii) $-x, y, \frac{3}{2} - z$.]

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(0.06 g, 0.2 mmol) after several days. CH&N analysis for $C_{20}H_{20}N_2O_8S_2$ (found/calc): C 50.00 (50.19), H 4.19 (4.31), N 5.83% (5.91%).

Crystal data

$C_{10}H_{10}N_2^{2+} \cdot C_{10}H_6O_6S_2^{2-} \cdot 2H_2O$	$D_x = 1.572$ Mg m^{-3}
$M_r = 480.50$	Mo $K\alpha$ radiation
Monoclinic, $P2/c$	Cell parameters from 1542
$a = 9.8121$ (9) Å	reflections
$b = 6.6775$ (6) Å	$\theta = 2.7–27.1°$
$c = 15.647$ (1) Å	$\mu = 0.32$ mm^{-1}
$\beta = 97.957$ (2)°	$T = 298$ (2) K
$V = 1015.3$ (2) Å^3	Plate, colorless
$Z = 2$	$0.27 \times 0.13 \times 0.08$ mm

Data collection

Bruker SMART APEX area-detector diffractometer	1860 reflections with $I > 2\sigma(I)$
	$R_{int} = 0.025$
φ and ω scans	$\theta_{max} = 27.5°$
Absorption correction: none	$h = -12 \rightarrow 5$
5865 measured reflections	$k = -8 \rightarrow 8$
2296 independent reflections	$l = -20 \rightarrow 20$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0721P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.049$	$+ 0.203P]$
$wR(F^2) = 0.134$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} = 0.001$
2296 reflections	$\Delta\rho_{max} = 0.23$ e Å^{-3}
157 parameters	$\Delta\rho_{min} = -0.40$ e Å^{-3}
H atoms treated by a mixture of independent and constrained refinement	

Table 1
Selected geometric parameters (Å, °).

S1—O1	1.449 (2)	C3—C4	1.356 (3)
S1—O2	1.454 (2)	C4—C5	1.422 (3)
S1—O3	1.440 (2)	C5—C5^i	1.430 (4)
S1—C1	1.787 (2)	C6—C7	1.376 (3)
N1—C6	1.321 (3)	C7—C8	1.394 (3)
N1—C10	1.325 (3)	C8—C9	1.381 (3)
C1—C2	1.367 (3)	C8—C8^{ii}	1.480 (4)
C1—C5^i	1.433 (3)	C9—C10	1.380 (3)
C2—C3	1.408 (3)		
O1—S1—O2	112.1 (1)	C3—C4—C5	121.3 (2)
O1—S1—O3	113.0 (1)	C4—C5—C5^i	118.8 (2)
O2—S1—O3	112.1 (1)	C4—C5—C1^i	123.3 (2)
O1—S1—C1	105.8 (1)	C5^i—C5—C1^i	117.9 (2)
O2—S1—C1	106.3 (1)	N1—C6—C7	120.7 (2)
O3—S1—C1	107.0 (1)	C6—C7—C8	119.0 (2)
C6—N1—C10	122.2 (2)	C9—C8—C7	118.3 (2)
C2—C1—C5^i	121.3 (2)	C9—C8—C8^{ii}	120.6 (2)
C2—C1—S1	117.4 (2)	C7—C8—C8^{ii}	121.0 (3)
C5^i—C1—S1	121.3 (2)	C10—C9—C8	119.9 (2)
C1—C2—C3	120.0 (2)	N1—C10—C9	119.9 (2)
C4—C3—C2	120.7 (2)		

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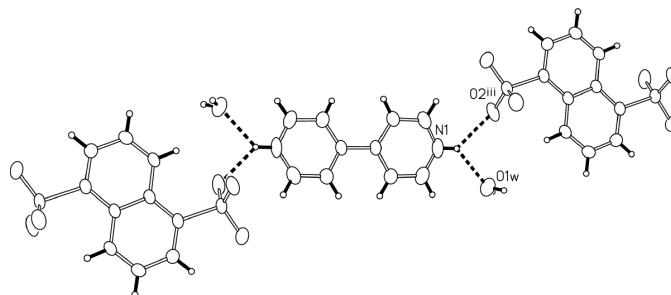

Figure 2
*ORTEP*II (Johnson, 1976) plot illustrating the bifurcated pyridinium hydrogen bond (dashed lines). [Symmetry code (iii) $1 - x, 1 - y, 1 - z$.]

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

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1w—H1w1$\cdots$O1	0.85 (1)	2.00 (1)	2.832 (3)	167 (3)
O1w—H1w2$\cdots$O2^{iv}	0.84 (1)	1.99 (1)	2.826 (2)	176 (3)
N1—H1$n\cdots$O1w	0.86 (1)	2.16 (2)	2.810 (3)	133 (2)
N1—H1$n\cdots$O2^{iii}	0.86 (1)	2.22 (2)	2.885 (2)	134 (2)

Symmetry codes: (iii) $1 - x, 1 - y, 1 - z$; (iv) $x, y - 1, z$.

The aromatic H atoms were placed at calculated positions [C—H 0.93 Å; $U(H) = 1.2U_{eq}(C)$] in the riding-model approximation. The water and pyridinium H atoms were located and refined with a distance restraint of 0.85 (1) Å.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); 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: *ORTEP*II (Johnson, 1976); software used to prepare material for publication: *SHELXL*97.

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