Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

Bis(2-hydroxypyridinium) naphthalene-1,5-disulfonate dihydrate

Shan Gao,[a] Li-Hua Huo[a] and Seik Weng Ng[b]*

[a]College of Chemistry and Chemical Technology, Heilongjiang University, Harbin 150080, People's Republic of China, and [b]Department of Chemistry, University of Malaya, Kuala Lumpur 50603, Malaysia

Correspondence e-mail: seikweng@um.edu.my

Received 25 October 2004
Accepted 7 December 2004
Online 11 December 2004

The cation, anion and water molecules of the title compound, $2C_5H_6NO^+\cdot C_{10}H_6O_6S_2^{2-}\cdot 2H_2O$, interact *via* hydrogen bonds, giving rise to a tight three-dimensional network structure. Two independent anions both lie on centers of inversion, and the asymmetric unit consists of two half-anions, two independent cations and two independent water molecules.

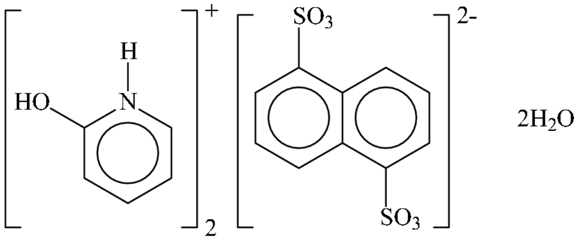
Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.044
wR factor = 0.123
Data-to-parameter ratio = 15.0

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

Comment

The rigid naphthalenedisulfonate dianion furnishes a number of coordination sites for binding to metal ions (Cai, 2004).



(I)

The dianion has been isolated as the anhydrous ammonium, 1-(hydroxymethyl)-3,5,7-triaza-1-azoniatricyclo[3.3.1.13,7]-decane (Sakwa & Wheeler, 2003) and hydrated thiamine (Shin & Lah, 1987) salts. Probably because the 2-hydroxypyridinium salt has fewer donor sites, the compound crystallizes with two water molecules per formula unit, (I) (Fig. 1). The asymmetric unit consists of two half-anions (the anions lying on centers of inversion), two cations and two water molecules. The structure has extensive hydrogen bonds (Table 1) that consolidate it in a three-dimensional network. The 2-hydroxypyridinium cation shows a lengthening of the carbon–oxygen bond [1.307 (2) Å] relative to that [1.251 (1) Å] in the parent compound, which is formally a pyridinone (Yang & Craven, 1998).

Experimental

Nickel diacetate tetrahydrate (0.50 g, 2 mmol) and 2-hydroxypyridine (0.19 g, 3 mmol) were added to an aqueous solution of sodium naphthalene-1,5-disulfonate (1.00 g, 3 mmol). Colorless crystals of the organic salt separated from the solution after several days. Analysis calculated: C 62.15, H 5.74, N 7.25%; found: C 62.01, H 5.68, N 7.31%.

doi:10.1107/S1600536804032313

Crystal data

$2C_5H_6NO^+ \cdot C_{10}H_6O_6S_2^{2-} \cdot 2H_2O$
$M_r = 514.52$
Monoclinic, $P2_1/c$
$a = 14.740$ (3) Å
$b = 10.883$ (2) Å
$c = 14.075$ (3) Å
$\beta = 96.91$ (3)°
$V = 2241.7$ (8) Å^3
$Z = 4$
$D_x = 1.525$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 16 290 reflections
$\theta = 3.3$–27.4°
$\mu = 0.30$ mm^{-1}
$T = 295$ (2) K
Prism, colorless
0.42 × 0.31 × 0.24 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
ω scans
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
$T_{\min} = 0.797$, $T_{\max} = 0.932$
20 659 measured reflections
5082 independent reflections
3742 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.025$
$\theta_{\max} = 27.5°$
$h = -19 \rightarrow 19$
$k = -14 \rightarrow 12$
$l = -18 \rightarrow 18$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.044$
$wR(F^2) = 0.123$
$S = 1.03$
5082 reflections
339 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0679P)^2 + 0.5447P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.001$
$\Delta\rho_{\max} = 0.44$ e Å^{-3}
$\Delta\rho_{\min} = -0.21$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O7—H7O···O2w	0.86 (1)	1.65 (1)	2.509 (2)	179 (3)
O8—H8O···O1w	0.85 (1)	1.70 (1)	2.550 (2)	178 (3)
O1w—H1w1···O1	0.85 (1)	1.95 (1)	2.794 (2)	170 (2)
O1w—H1w2···O5$^{\rm i}$	0.85 (1)	2.06 (1)	2.854 (3)	154 (2)
O2w—H2w1···O4	0.85 (1)	1.97 (1)	2.803 (2)	168 (3)
O2w—H2w2···O3$^{\rm ii}$	0.85 (1)	1.95 (1)	2.782 (3)	168 (2)
N1—H1N···O2	0.86 (1)	1.86 (1)	2.700 (2)	165 (2)
N2—H2N···O5	0.85 (1)	1.92 (1)	2.748 (2)	167 (2)

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

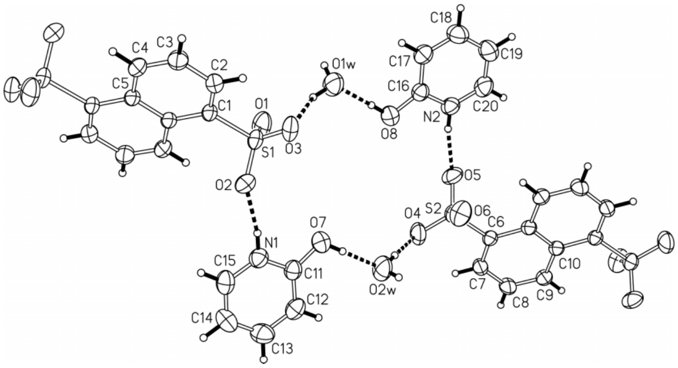


Figure 1
ORTEPII (Johnson, 1976) plot of (I), with displacement ellipsoids at the 50% probability level. H atoms are drawn as spheres of arbitrary radii. Dashed lines indicate hydrogen bonds.

The aromatic H atoms were placed in calculated positions [C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C)] and were included in the refinement in the riding-model approximation. The water and pyridinium H atoms were located and refined with distance restraints of O—H = N—H = 0.85 (1) Å and H···H = 1.39 (1) Å. The $h = 2n + 1$ reflections are all generally weak, and the refinement on a unit cell having an a axis half as long gave an identical residual index [for 2128 $I > 2\sigma(I)$ reflections]. The set of discarded 'non-fit' reflection indices had some relatively strong intensities although most were weak, *e.g.* 300 arbitrary units for the $\overline{3}30$ reflection compared with 1100 arbitrary units for the 020 reflection. The set of $h = 2n + 1$ excludes the possibility of a smaller unit cell.

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

We thank the National Natural Science Foundation of China (No. 20101003), the Scientific Fund for Remarkable Teachers of Heilongjiang Province (No. 1054 G036) and the University of Malaya for supporting this study.

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