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Key indicators

Single-crystal X-ray study
 $T = 295$ K
Mean $\sigma(\text{C}-\text{C}) = 0.004$ Å
Disorder in main residue
 R factor = 0.049
 wR factor = 0.160
Data-to-parameter ratio = 11.5For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.Bis[4-[(4-pyridyl)ethenyl]pyridinium}
4-sulfonatobenzoate trihydrate

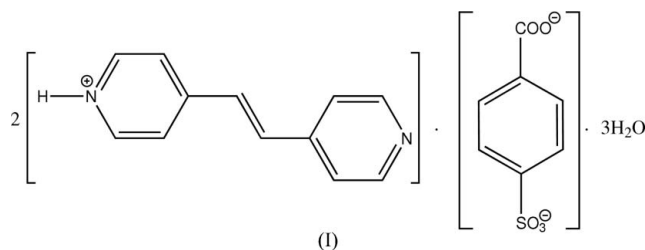
In the crystal structure of the title organic proton-transfer complex, $2\text{C}_{12}\text{H}_{11}\text{N}_2^+ \cdot \text{C}_7\text{H}_4\text{O}_5\text{S}^{2-} \cdot 3\text{H}_2\text{O}$, the cations form one-dimensional chains *via* intermolecular $\text{N}-\text{H} \cdots \text{N}$ hydrogen bonds and these chains, in turn, form a two-dimensional network through $\pi-\pi$ stacking interactions. In addition, the anions and water molecules are connected into a two-dimensional hydrogen-bonded network through intermolecular $\text{O}-\text{H} \cdots \text{O}$ hydrogen bonds. The two motifs result in sheets of cations and anions stacked alternately.

Received 13 March 2006

Accepted 15 March 2006

Comment

We have recently synthesized some 4-sulfobenzoate (sb) metal complexes exhibiting diverse topologies (Fan *et al.*, 2004; Zhang & Zhu, 2005; Zhang, Zhu & Ng, 2005), but there are no crystal structures of organic complexes with sb reported in the literature. We prepared a system of $\text{Pb}^{2+}/\text{sb}/1,10$ -phenanthroline under hydrothermal conditions, which gave a two-dimensional polymer with μ_4 -sb (Zhang, Zhu & Xiao, 2005). However, we unexpectedly prepared an organic complex, (I), using the 1,2-bis(4-pyridine)ethylene (bpe) ligand instead of 1,10-phenanthroline in the above procedure.



The title complex, (I), consists of two singly protonated bpe cations, a 4-sulfonatobenzoate dianion and three solvent water molecules (Fig. 1). The dihedral angles between the two pyridine rings of the Hbpe^+ cations are 10.7 (1) and 11.95 (9) $^\circ$ for the cations containing atoms N1 and N3, respectively. The protonated bpe species form one-dimensional $\text{N}-\text{H} \cdots \text{N}$ hydrogen-bonded chains and are further connected into sheets *via* $\pi-\pi$ stacking interactions between pyridine rings from adjacent chains. The centroid-centroid distances are 3.6024 (16), 3.6884 (17) and 3.6411 (18) Å, respectively, for $\text{Cg}1 \cdots \text{Cg}1^{\text{i}}$, $\text{Cg}2 \cdots \text{Cg}3^{\text{ii}}$ and $\text{Cg}4 \cdots \text{Cg}(4)^{\text{iii}}$ [where Cg1 is the centroid defined by atoms C1–C5/N1, Cg2 by C8–C12/N2, Cg3 by C13–C17/N3 and Cg4 by C20–C24/N2; symmetry codes: (i) $2-x, 1-y, 1-z$; (ii) $1-x, 1-y, -z$; (iii) $3-x, 1-y, -z$]. In addition, sb dianions and water molecules form a two-dimensional layer through extensive $\text{O}-\text{H} \cdots \text{O}$ interactions (Fig. 2 and Table 1). The two motifs result in sheets of cations and anions stacked alternately (Fig. 3).

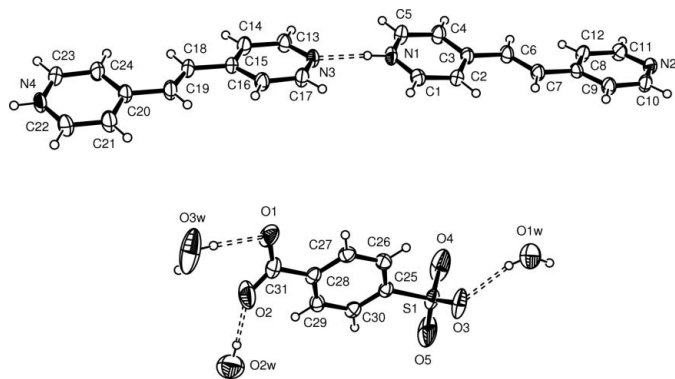


Figure 1
The asymmetric unit of (I), with displacement ellipsoids are drawn at the 40% probability level. Dashed lines indicate hydrogen bonds. The minor disorder component of the sulfonate group has been omitted for clarity.

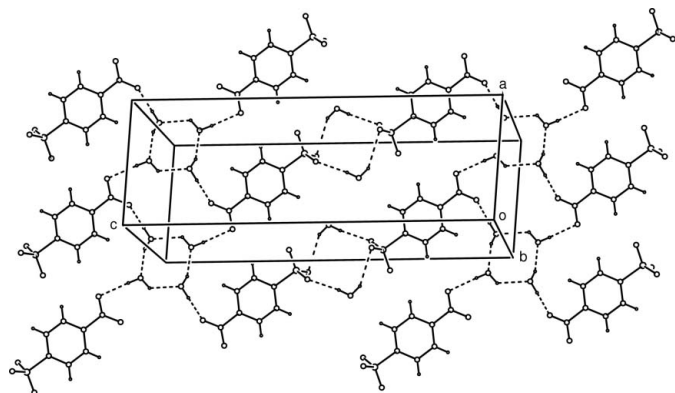


Figure 2
A view of the two-dimensional hydrogen-bonded anionic layer in (I), with hydrogen bonds shown as dashed lines. The minor disorder component of the sulfonate group has been omitted for clarity.

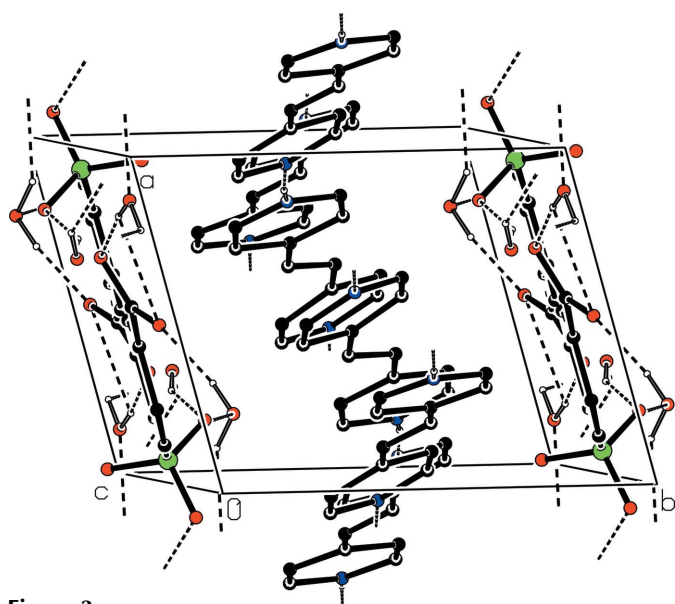


Figure 3
Packing plot (Spek, 2003) showing alternating sheets of hydrogen-bonded (dashed lines) sheets of anions and cations. Colour codes: green S, red O, blue N and black C. H atoms not involved in hydrogen bonding have been omitted.

Experimental

A mixture of $\text{Pb}(\text{NO}_3)_2$ (0.095 g, 0.29 mmol), potassium hydrogen 4-sulfobenzoate (0.060 g, 0.25 mmol), and 1,2-bis(4-pyridine)ethylene (0.045 g, 0.25 mmol) in an aqueous solution (15 ml) was sealed in a 25 ml stainless steel reactor with Teflon liner, and heated at 453 K for 24 h. When cooled to room temperature, a clear solution was obtained which was allowed to evaporate slowly. After 4 d, yellow block-shaped crystals of (I) were collected by suction filtration.

Crystal data

$2\text{C}_{12}\text{H}_{11}\text{N}_2^+ \cdot \text{C}_7\text{H}_4\text{O}_5\text{S}^{2-} \cdot 3\text{H}_2\text{O}$
 $M_r = 620.67$
 Triclinic, $P\bar{1}$
 $a = 7.4704$ (15) Å
 $b = 9.2406$ (18) Å
 $c = 22.121$ (4) Å
 $\alpha = 99.099$ (19)°
 $\beta = 94.823$ (14)°
 $\gamma = 103.471$ (17)°
 $V = 1454.7$ (5) Å³
 $Z = 2$

$D_x = 1.417$ Mg m⁻³
 Mo $K\alpha$ radiation
 Cell parameters from 6599 reflections
 $\theta = 3.1\text{--}27.5^\circ$
 $\mu = 0.17$ mm⁻¹
 $T = 295$ (2) K
 Block, yellow
 $0.41 \times 0.25 \times 0.18$ mm

Data collection

Rigaku R-Axis RAPID diffractometer
 ω scans
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)
 $T_{\text{min}} = 0.933$, $T_{\text{max}} = 0.972$
 11622 measured reflections

5156 independent reflections
 3874 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.019$
 $\theta_{\text{max}} = 25.1^\circ$
 $h = -8 \rightarrow 8$
 $k = -11 \rightarrow 11$
 $l = -26 \rightarrow 26$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.160$
 $S = 1.10$
 5156 reflections
 449 parameters
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1022P)^2 + 0.0982P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.49$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.43$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D\text{---}H\cdots A$	$D\text{---}H$	$H\cdots A$	$D\cdots A$	$D\text{---}H\cdots A$
$\text{N1---H1A}\cdots\text{N3}$	0.83 (1)	1.92 (1)	2.742 (3)	174 (4)
$\text{N4---H4A}\cdots\text{N2}^i$	0.83 (1)	1.85 (1)	2.683 (3)	175 (3)
$\text{O1W---H1C}\cdots\text{O5}^{iii}$	0.85 (1)	2.07 (1)	2.906 (8)	170 (3)
$\text{O1W---H1C}\cdots\text{O5}^{ii}$	0.85 (1)	2.28 (2)	3.057 (7)	152 (3)
$\text{O1W---H1C}\cdots\text{O4}^{ii}$	0.85 (1)	2.62 (2)	3.384 (7)	150 (3)
$\text{O1W---H1B}\cdots\text{O3}$	0.85 (1)	2.12 (2)	2.916 (5)	157 (4)
$\text{O1W---H1B}\cdots\text{O4}^i$	0.85 (1)	2.15 (2)	2.946 (14)	156 (4)
$\text{O2W---H2A}\cdots\text{O3W}^{iii}$	0.87 (3)	1.91 (2)	2.695 (5)	150 (3)
$\text{O3W---H3A}\cdots\text{O2W}^{iv}$	0.86 (3)	2.18 (3)	2.774 (5)	126 (3)
$\text{O3W---H3B}\cdots\text{O1}$	0.85 (3)	2.05 (3)	2.899 (4)	175 (4)
$\text{O3W---H3B}\cdots\text{O2}$	0.85 (3)	2.55 (3)	3.075 (4)	121 (2)
$\text{O2W---H2B}\cdots\text{O2}$	0.87 (3)	1.82 (3)	2.677 (4)	171 (3)

Symmetry codes: (i) $x+1, y, z-1$; (ii) $-x, -y+2, -z+1$; (iii) $x-1, y, z$; (iv) $-x+1, -y+2, -z$.

H atoms bonded to C atoms were placed in idealized positions and refined as riding atoms, with $\text{C---H} = 0.93$ Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$. H atoms bound to O and N atoms were located in difference Fourier maps and refined with distance restraints of $\text{O---H} = 0.85$ (1) Å and $\text{N---H} = 0.82$ (1) Å, and fixed isotropic displacement parameter of $U_{\text{iso}}(\text{H}) = 0.08$ Å². The sulfonate O atoms are disordered over two

positions in the ratio 0.685 (7):0.315 (7) for atoms O3/O4/O5 and O3'/O4'/O5', respectively.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSK, 2002); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

The authors thank Heilongjiang University for the diffraction measurements, the National Natural Science Foundation of China (grant No. 50073019) and the Analytical and Measurement Fund of Zhejiang Province.

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