2-[(E)-2-(4-Methoxyphenyl)ethenyl]-1-methyl-quinolinium 4-methoxybenzenesulfonate monohydrate

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In the title compound, $C_{19}H_{18}NO^+ \cdot C_7H_7O_4S^- \cdot H_2O$, the cation adopts an E configuration and is almost planar. The quinolinium group and benzene ring of the cation make dihedral angles of 84.40 (8) and 85.80 (11)°, respectively, with the benzene ring of the anion. The crystal structure is stabilized by intermolecular O—H⋯O hydrogen bonds together with weak intra- and intermolecular C—H⋯O interactions. The cations are arranged in one-dimensional chains along the b axis and these chains are interconnected with the anions through weak C—H⋯O interactions. The water molecules are also hydrogen-bonded to the anions to form a three-dimensional network. C—H⋯π interactions are also observed in the crystal structure.

Comment

Designing a new material for nonlinear optics (NLO) demands both molecular and crystal characterization of the promising compound. Our continuing research on NLO materials (Jindawong, Chantrapromma, Fun, Yu & Karalai, 2005; Jindawong, Chantrapromma, Fun & Karalai, 2005; Chantrapromma et al., 2005, 2006; Fun et al., 2006) has led us to synthesize the title compound, (I), with the aim of exploring its structure and crystal packing in order to gain further information on the effect of the counter-anion on the crystal packing and on the NLO properties of the compound. Second-order nonlinear effects require a non-centrosymmetric structure for the bulk material (Williams, 1984). However, since compound (I) crystallizes in the centrosymmetric space group $P2_1/c$, it does not exhibit second-order NLO properties.

(I)
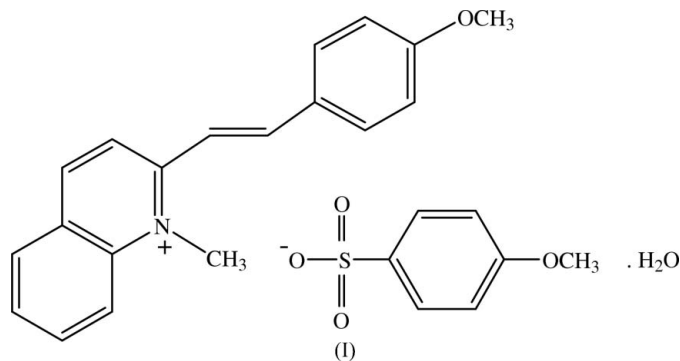
The asymmetric unit of (I) consists of a $C_{19}H_{18}NO^+$ cation, a $C_7H_7SO_4^-$ anion and an H_2O molecule (Fig. 1). Bond lengths and angles are in normal ranges (Allen et al., 1987) and similar to those in some closely related structures, such as 2-[(E)-2-(3-hydroxy-4-methoxyphenyl)ethenyl]-1-methylquinolinium   4-
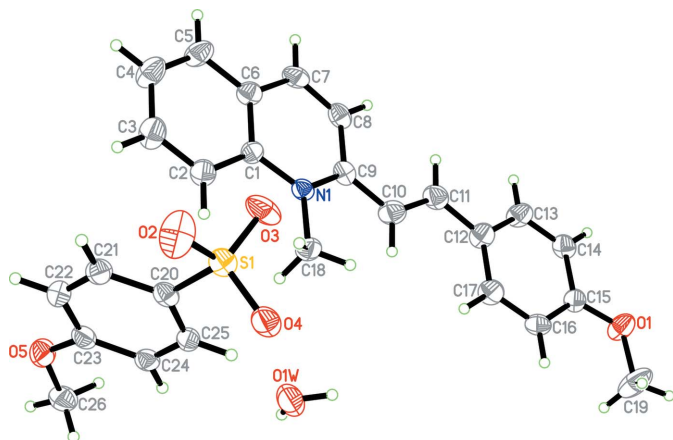
Figure 1
The asymmetric unit of (I), showing 60% probability displacement ellipsoids and the atomic numbering scheme.
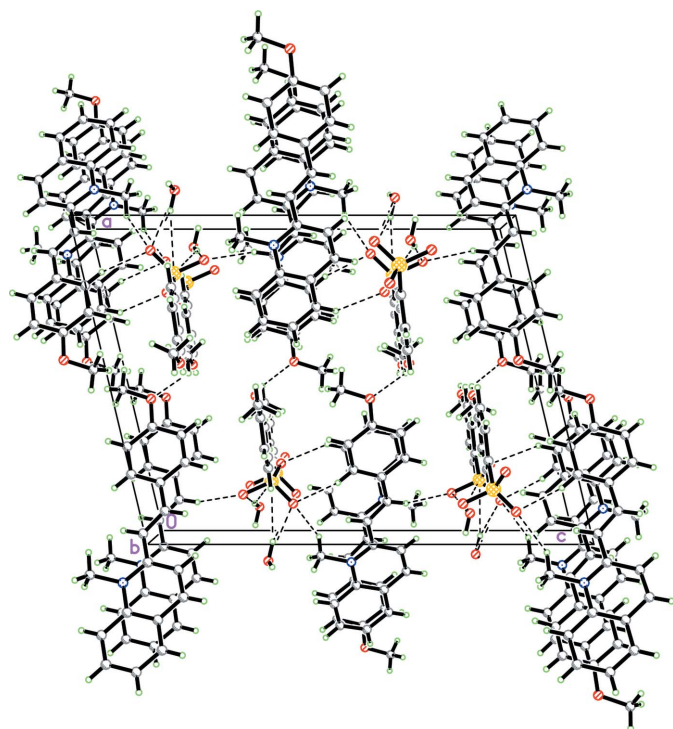
Figure 2
The crystal packing of (I), viewed down the b axis. The O—H···O hydrogen bonds and weak C—H···O interactions are shown as dashed lines.

methylbenzenesulfonate, (II) (Jindawong, Chantrapromma, Fun & Karalai, 2005), 2-[(E)-2-(3-hydroxy-4-methoxyphenyl)ethenyl]-1-methylquinolinium 4-chlorobenzenesulfonate, (III) (Chantrapromma *et al.*, 2006), and 2-[(E)-2-(4-methoxyphenyl)ethenyl]-1-methylquinolinium 4-bromobenzenesulfonate, (IV) (Fun *et al.*, 2006).

In the cation of (I), the quinolinium group (C1–C9/N1) is planar, with a maximum deviation from the plane of 0.062 (2) Å for atom N1. Overall, the cation is almost planar, as indicated by the dihedral angle of 3.92 (10)° between the quinolinium group and the C12–C17 benzene ring [2.59 (9)° in (II), 2.8 (1)° in (III) and 1.12 (14)° in (IV)]. The cation adopts

an E configuration, the C9—C10—C11—C12 torsion angle being 179.6 (2)°. The O1—C19 methoxy group lies almost in the plane of the benzene ring of the cation, with C19—O1—C15—C16 = −1.1 (3)°, whereas the O5—C26 methoxy group in the anion is slightly twisted from the C20–C25 benzene plane, with C26—O5—C23—C22 = −174.22 (19)°.

In the asymmetric unit, the cation and anion are almost perpendicular to each other, with a dihedral angle of 84.40 (8)° between the benzene ring of the anion and the quinolinium plane. This can be compared with 59.17 (9)° in (II) and 48.97 (6)° in (III), and 84.23 (12)° in (IV). The dihedral angle between the benzene rings of the anion and cation is 85.80 (11)° [60.59 (10)° in (II) and 51.63 (7)° in (III), and 84.59 (15)° in (IV)].

The cations of (I) are arranged into one-dimensional chains along the b axis. The cationic chains are stacked in an antiparallel manner down the a axis into a cationic sheet. These cationic sheets are interconnected with the anions through weak C—H···O interactions. The water molecules are also hydrogen-bonded to 4-methoxybenzenesulfonate anions to form a three-dimensional molecular network. C—H···π interactions are also observed (Table 2, Fig. 2; $Cg1$ is the centroid of the C20–C25 benzene ring).

Experimental

2-(4′-Methoxystyryl)-1-methylquinolinium iodide (compound A) was synthesized according to our previously reported method (Fun *et al.*, 2006). Silver(I) 4-methoxybenzenesulfonate (Compound B) was prepared by mixing a solution (1:2:1 molar ratio) of 4-methoxybenzenesulfonyl chloride (2.48 g, 12 mmol), sodium hydroxide (0.96 g, 24 mmol) and silver nitrate (2.04 g, 12 mmol) in hot CH₃OH (60 ml). The mixture was stirred for *ca* 10 min and then filtered. The resulting colourless solution was evaporated to yield a white compound, B (m.p. 516–518 K). Compound (I) was synthesized by mixing solutions of A (0.10 g, 0.25 mmol) and B (0.07 g, 0.25 mmol) each in hot CH₃OH (50 ml), which immediately gave a yellow mass of silver iodide. After stirring the mixture for 30 min, the silver iodide was removed by filtration and the resulting green–yellow solution evaporated to yield a yellow solid. Single yellow plates of (I) were obtained by recrystallization from CH₃OH at ambient temperature over several days (m.p. 500–502 K).

Crystal data

$C_{19}H_{18}NO^+ \cdot C_7H_7O_4S^- \cdot H_2O$	$Z = 4$
$M_r = 481.55$	$D_x = 1.401$ Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
$a = 14.6155$ (2) Å	$\mu = 0.19$ mm^{-1}
$b = 8.3133$ (1) Å	$T = 100.0$ (1) K
$c = 19.3131$ (2) Å	Plate, yellow
$\beta = 103.401$ (1)°	$0.27 \times 0.25 \times 0.08$ mm
$V = 2282.71$ (5) Å^3	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	41723 measured reflections
ω scans	5509 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	4300 reflections with $I > 2\sigma(I)$
$T_{min} = 0.951$, $T_{max} = 0.986$	$R_{int} = 0.046$
	$\theta_{max} = 28.0°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.154$
$S = 1.04$
5509 reflections
318 parameters
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0766P)^2 + 2.0189P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.81$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ e Å^{-3}

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

$Cg1$ is the centroid of the C20–C25 benzene ring.

$D-\mathrm{H}\cdots A$	$D-\mathrm{H}$	$\mathrm{H}\cdots A$	$D\cdots A$	$D-\mathrm{H}\cdots A$
O1W—H1W1···O2[i]	0.89 (4)	2.58 (4)	3.116 (3)	120 (3)
O1W—H1W1···O3[i]	0.89 (4)	2.27 (4)	3.162 (3)	179 (3)
O1W—H2W1···O4[ii]	0.90 (4)	1.99 (4)	2.860 (3)	163 (4)
C5—H5A···O2[iii]	0.93	2.42	3.245 (3)	148
C7—H7A···O1W[iv]	0.93	2.58	3.371 (3)	143
C11—H11A···O3[v]	0.93	2.47	3.373 (3)	163
C17—H17A···O4[ii]	0.93	2.37	3.281 (3)	165
C18—H18A···O4[ii]	0.96	2.45	3.289 (3)	147
C21—H21A···O2	0.93	2.53	2.895 (3)	104
C26—H26A···O1[vi]	0.96	2.57	3.307 (3)	134
C2—H2A···$Cg1$	0.93	2.88	3.673 (2)	144
C16—H16A···$Cg1$[ii]	0.93	2.90	3.793 (2)	161

Symmetry codes: (i) $x, y+1, z$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iv) $x, -y+\frac{3}{2}, z-\frac{1}{2}$; (v) $-x, -y+1, -z$; (vi) $x+1, -y+\frac{5}{2}, z+\frac{1}{2}$.

Water H atoms were located in a difference map and refined isotropically (distances are in Table 1). All H atoms bound to carbon were refined using a riding model, with C—H = 0.93 Å and $U_{iso}(\mathrm{H}) = 1.2U_{eq}(\mathrm{C})$ for aromatic H, and C—H = 0.96 Å and $U_{iso}(\mathrm{H}) = 1.5U_{eq}(\mathrm{C})$ for CH$_3$ atoms. A rotating-group model was used for the CH$_3$ groups.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

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