organic papers

2-[(*E*)-2-(3-Hydroxy-4-methoxyphenyl)-ethenyl]-1-methylquinolinium 0.59-chloride 0.41-iodide monohydrate

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The title compound, $C_{19}H_{18}NO_2^+ \cdot 0.59\,Cl^- \cdot 0.41\,I^- \cdot H_2O$, exhibits second-order non-linear optical properties. The cations are essentially planar and they are linked with water molecules through O—H···O hydrogen bonds, and the water molecules are linked with Cl^- ions by O—H···Cl hydrogen bonds, forming infinite chains of chloride salts along the *a* axis.

Comment

The crystalline state is, in principle, the best medium for generating non-linear optical (NLO) phenomena because of the high packing density of the active components. The structure analysis of the title compound, (I), has been undertaken as part of our ongoing crystallographic investigations of NLO materials (Rahman *et al.*, 2003; Jindawong, Chantrapromma, Fun, Yu & Karalai, 2005; Jindawong, Chantrapromma, Fun & Karalai, 2005; Chantrapromma *et al.*, 2005; 2006). Compound (I) crystallized in the non-centrosymmetric space group *P*1 and so exhibits second-order NLO properties (Williams, 1984). Moreover, molecules of (I) are packed in a parallel fashion in a non-centrosymmetric space group which is one of the requirements for good NLO materials (Hulliger *et al.*, 1998).

(I)
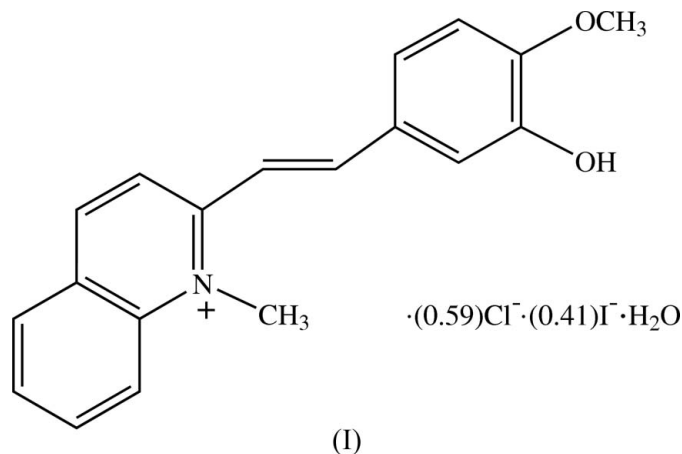
The refinement of (I) revealed the composition to be $C_{19}H_{18}NO_2^+ \cdot 0.59\,Cl^- \cdot 0.41\,I^- \cdot H_2O$ (Fig. 1), *i.e.* with fractional occupancy of the halide ions. The bond distances and angles in (I) have normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Jindawong, Chantrapromma, Fun, Yu & Karalai, 2005; Jindawong, Chantrapromma, Fun & Karalai, 2005; Chantrapromma *et al.*, 2005; 2006). The cation is essentially planar, the dihedral angles between the two aromatic (C1–C6 and C12–C17) rings being 1.6 (3)°. The methoxy group is almost coplanar with the attached aromatic
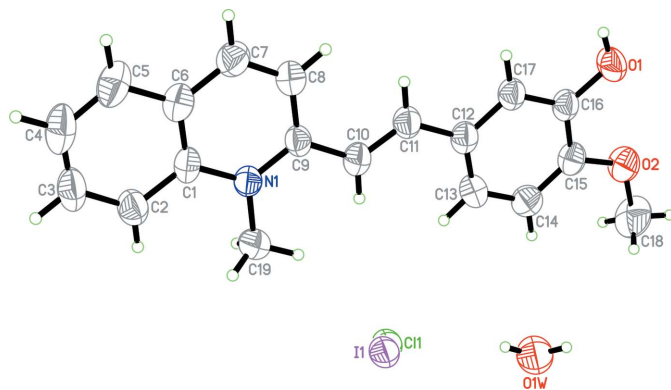
Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering.
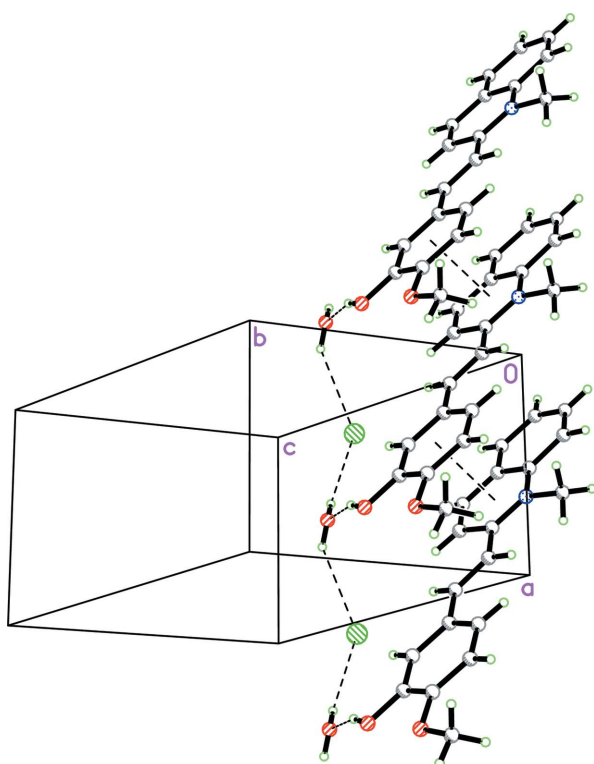

Figure 2
The crystal packing for the chloride salt of (I), viewed down the *c* axis. Hydrogen bonds and π–π interactions are shown as dashed lines.

ring, as indicated by the C18—O2—C15—C16 and C13—C14—C15–O2 torsion angles of 176.3 (4) and 179.1 (4)°, respectively.

Intermolecular O—H···O, intra- and intermolecular O—H···Cl and weaker C—H···O hydrogen-bonding interactions are observed in the crystal structure of (I) (Table 1). Cations are linked with water molecules through O—H···O hydrogen bonds, and the water molecules are linked with Cl⁻ ions by O—H···Cl hydrogen bonds, forming infinite chains of the chloride salt along the *a* axis (Fig. 2). Within the chains, there is a centroid–centroid distance of 3.640 (2) Å between the N1/C1/C6–C9 ring and the C12–C17 ring at (−1 + *x*, *y*, *z*), indicating π–π interactions (Fig. 2). The iodide salt is not linked

into infinite chains as the equivalent O—H···I hydrogen bonds are not formed, the O···I distances being greater than 3.60 Å.

Experimental

The title compound, (I), is a by-product of our first attempt to synthesize the NLO compound 2-[(E)-2-(3-hydroxy-4-methoxy-phenyl)ethenyl]-1-methylquinolinium 4-chlorobenzenesulfonate (Chantrapromma *et al.*, 2006). The preparation of (I) was synthesized following the same procedure as previously reported (Chantrapromma *et al.*, 2006) by mixing a solution of 2-(4-methoxy-3-hydroxystyryl)-1-methylquinolinium iodide (0.28 g, 0.67 mmol) and silver (I) 4-chlorobenzenesulfonate (0.20 g, 0.67 mmol) in hot methanol (50 ml). The mixing immediately yielded a yellow solid of silver iodide. The silver iodide precipitate was removed and the resulting solution was evaporated, yielding a solid powder. The resulting solid was washed with chloroform and recrystallized from methanol, giving colorless needles of (I) after a few weeks (m.p. 478–480 K).

Crystal data

$C_{19}H_{18}NO_2^+ \cdot 0.59Cl^- \cdot 0.41I^- \cdot H_2O$	$V = 439.41 (7)$ Å^3
$M_r = 383.49$	$Z = 1$
Triclinic, $P1$	$D_x = 1.449$ Mg m^{-3}
$a = 6.2645 (6)$ Å	Mo $K\alpha$ radiation
$b = 8.2382 (8)$ Å	$\mu = 0.89$ mm^{-1}
$c = 9.1458 (8)$ Å	$T = 153.0 (1)$ K
$\alpha = 68.743 (2)°$	Needle, colorless
$\beta = 88.273 (1)°$	$0.52 \times 0.11 \times 0.10$ mm
$\gamma = 87.467 (1)°$	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	6398 measured reflections
ω scans	3964 independent reflections
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	3677 reflections with $I > 2\sigma(I)$
$T_{min} = 0.661$, $T_{max} = 0.920$	$R_{int} = 0.017$
	$\theta_{max} = 28.0°$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0738P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.048$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.125$	$(\Delta/\sigma)_{max} = 0.003$
$S = 1.16$	$\Delta\rho_{max} = 1.14$ e Å^{-3}
3964 reflections	$\Delta\rho_{min} = -0.28$ e Å^{-3}
224 parameters	Absolute structure: Flack (1983), 1853 Freidel pairs
H-atom parameters constrained	Flack parameter: −0.04 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O1W^i	0.82	1.88	2.671 (5)	161
O1W—H1W1···Cl1^{ii}	0.85	2.78	3.51 (2)	145
O1W—H2W1···Cl1	0.85	2.78	3.59 (2)	161
C3—H3···O1^{iii}	0.93	2.59	3.254 (6)	129
C19—H19C···O2^{iv}	0.96	2.59	3.433 (7)	146

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

Water-bound H atoms were located using *WinGX* (Farrugia, 1999) and then refined as riding on the O1W atom. The remaining H atoms were placed in calculated positions, with an O—H distance of 0.82 Å

and C—H distances in the range 0.93–0.96 Å. The U_{iso}(H) values were constrained to $1.5U_{eq}$ of the carrier atom for hydroxyl and methyl H atoms, and $1.2U_{eq}$(C) for the remaining H atoms. A rotating group model was used for the methyl groups. The maximum residual electron density peak is located 1.11 Å from the I1 ion. The site occupancy factors for the chloride and iodide ions refined to 0.588 (4) and 0.412 (4), respectively.

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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