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

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.015
wR factor = 0.037
Data-to-parameter ratio = 31.3

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

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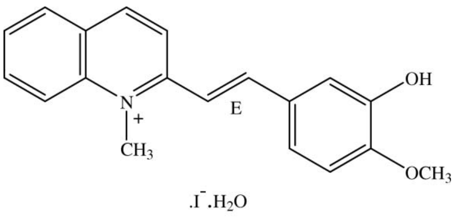
The title compound, $C_{19}H_{18}NO_2^+ \cdot I^- \cdot H_2O$, crystallizes in a non-cenrosymmetric space group and exhibits a non-linear optical property. The second-harmonic generation (SHG) efficiency is about 1.95 times that of urea. The cation is essentially planar. The water molecules and anions are linked into a chain along the *a* axis by $O_{water}—H\cdots I$ hydrogen bonds, and the cations are linked to it *via* $O—H\cdots O_{water}$ hydrogen bonds. In addition, π–π and $C—H\cdots O$ interactions are observed.

Comment

The search for new non-linear optical (NLO) materials showing large macroscopic susceptibilities has attracted a great deal of attention owing to their interesting applications (Prasad & Williams, 1991; Chemla & Zyss, 1987). The most important criterion for a single crystal to exhibit second-order NLO properties is that the molecules have to be oriented in a non-centrosymmetric environment (Williams, 1984). In our continuing systematic study of NLO materials (Chantrapromma *et al.*, 2005, 2006; Fun *et al.*, 2006; Jindawong, Chantrapromma, Fun & Karalai, 2005; Jindawong, Chantrapromma, Fun, Yu & Karalai, 2005), we report here the crystal structure of the title compound, (I). Compound (I) crystallizes in a non-centrosymmetric space group, *P*1, and exhibits a second harmonic generation (SHG) effect. Powder SHG measurement (Kurtz & Perry, 1968) of (I) showed a conversion efficiency 1.95 times that of a urea standard.



(I)

The asymmetric unit of (I) consists of a $C_{19}H_{18}NO_2^+$ cation, an I^- anion and a water molecule (Fig. 1). The bond distances and angles in the cation have normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Jindawong, Chantrapromma, Fun & Karalai, 2005; Chantrapromma *et al.*, 2006; Fun *et al.*, 2006). The cation is essentially planar, with a maximum deviation of 0.030 (1) Å for C2. The H atoms attached to C10═C11 are *trans* to each other; thus the cation exists in an *E* configuration [the C9—C10—C11—C12 torsion angle is 179.35 (11)°]. The dihedral angle between the benzene and quinolinium ring systems is 1.21 (5)°.

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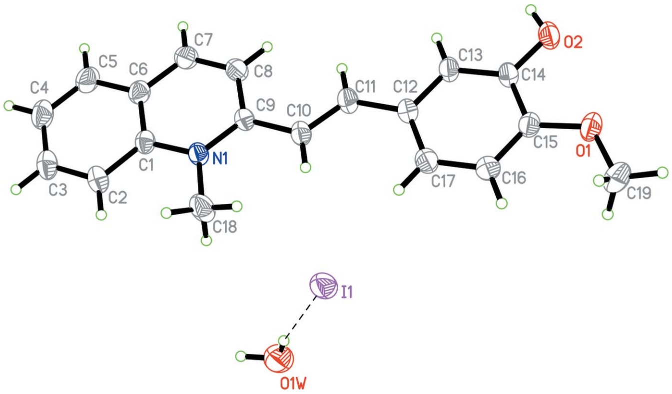

Figure 1
The asymmetric unit of (I), showing 80% probability displacement ellipsoids and the atomic numbering. The dashed line indicates an $O_{water}—H\cdots I$ hydrogen bond.

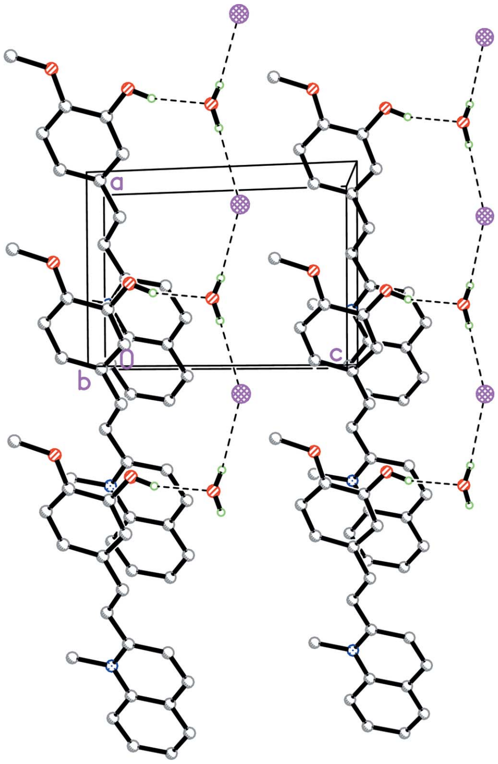

Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines. For clarity, H atoms not involved in the hydrogen bonds have been omitted.

The crystal packing (Fig. 2) shows that the water molecules and anions are linked into a chain along the *a* axis by $O_{water}—H\cdots I$ hydrogen bonds (Table 1). The cations are linked to the anionic chains through $O—H\cdots O$ hydrogen bonds involving the hydroxyl group and water molecules. Along the chain, the N1/C1/C6–C9 pyridine ring (centroid *Cg*1) and the C12–C17 benzene ring (centroid *Cg*2) of the adacent cations are stacked with a $Cg1\cdots Cg2(-1 + x, y, z)$ distance of 3.6305 (7) Å, indicating π–π interactions. The adjacent chains are cross-linked *via* $C—H\cdots O$ interactions (Table 1).

Experimental

Compound (I) was prepared by the condensation reaction of 1,2-dimethylquinolinium iodide (3.0 g, 10.05 mmol) and isovanillin (1.60 g, 10.05 mmol) in the presence of piperidine (1.00 ml, 10.00 mmol) in methanol (40 ml). The reaction mixture was refluxed for 2 h under a nitrogen atmosphere. The solid formed was filtered off, washed with diethyl ether and recrystallized from methanol to obtain block-shaped yellow single crystals of (I) (m.p. 491–493 K).

Crystal data

$C_{19}H_{18}NO_2^+\cdot I^-\cdot H_2O$
$M_r = 437.26$
Triclinic, $P1$
$a = 6.2412$ (1) Å
$b = 8.2854$ (2) Å
$c = 9.1961$ (2) Å
$\alpha = 68.134$ (1)°
$\beta = 89.424$ (1)°
$\gamma = 87.720$ (1)°
$V = 440.97$ (2) Å^3
$Z = 1$
Mo $K\alpha$ radiation
$\mu = 1.83$ mm^{-1}
$T = 100.0$ (1) K
0.55 × 0.50 × 0.41 mm

Data collection

Bruker SMART APEX II CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{min} = 0.433$, $T_{max} = 0.524$ (expected range = 0.390–0.472)
17774 measured reflections
7236 independent reflections
7233 reflections with $I > 2\sigma(I)$
$R_{int} = 0.017$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.015$
$wR(F^2) = 0.037$
$S = 1.09$
7236 reflections
231 parameters
4 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 1.12$ e Å^{-3}
$\Delta\rho_{min} = -0.59$ e Å^{-3}
Absolute structure: Flack (1983), 3382 Friedel pairs
Flack parameter: 0.012 (7)

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

$D—H\cdots A$	$D—H$	$H\cdots A$	$D\cdots A$	$D—H\cdots A$
$O2—H1O2\cdots O1W^{i}$	0.82 (3)	1.92 (3)	2.7086 (15)	163 (4)
$O1W—H1W\cdots I1^{ii}$	0.89 (6)	2.77 (5)	3.6584 (12)	174 (5)
$O1W—H2W\cdots I1$	0.84 (4)	2.78 (4)	3.6005 (12)	170 (4)
$C3—H3\cdots O2^{iii}$	0.93	2.51	3.1840 (16)	129

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

The hydroxyl and water H atoms were located in a difference Fourier map and refined isotropically. After checking their presence in a difference map, the C-bound H atoms were placed in calculated positions (C—H = 0.93 or 0.96 Å) and constrained to ride on their parent atoms with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$(methyl C). A rotating group model was used for the methyl groups. As the refinement resulted in a very short $H10\cdots H18C$ contact of 1.78 Å, the $H10\cdots H18C$ distance was restrained to 1.93 (1) Å. The highest residual electron density peak is located 0.69 Å from atom I1.

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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