Acta Crystallographica Section E
Structure Reports
Online

ISSN 1600-5368

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

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Received 20 March 2007
Accepted 24 March 2007

Key indicators

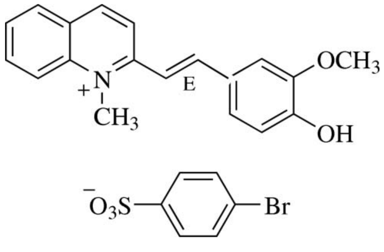
Single-crystal X-ray study
T = 297 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.090
Data-to-parameter ratio = 13.6

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

The title compound, $C_{19}H_{18}NO_2^+\cdot C_6H_4BrO_3S^-$, crystallizes in a non-centrosymmetric space group and exhibits a non-linear optical property. The second-harmonic generation (SHG) efficiency of the compound is about 0.8 times that of urea. The cation is almost planar. The cations and anions are arranged in alternating layers parallel to the *ab* plane, and these layers are interconnected through O—H⋯O and C—H⋯O interactions, forming a three-dimensional network.

Comment

The title compound, (I), was synthesized as part of our continuing research on the non-linear optical (NLO) properties of pyridinium and quinolinium derivatives (Chantrapromma *et al.*, 2005, 2006, 2007; Jindawong *et al.*, 2005; Fun *et al.*, 2006; Ruanwas *et al.*, 2007). By changing the anion from 4-methylbenzenesulfonate (Jindawong *et al.*, 2005) to 4-bromobenzenesulfonate in this work, the space group has changed from $P2_1/n$ (Jindawong *et al.*, 2005) to the non-centrosymmetric space group *Pc* in (I). The second-harmonic generation (SHG) efficiency of the (I) was measured by the standard powder technique (Kurtz & Perry, 1968). The SHG effect of the crystal of (I) is estimated to be about 0.8 times that of urea.



(I)

The asymmetric unit of (I) consists of a 2-[(*E*)-2-(3-hydroxy-4-methoxyphenyl)ethenyl]-1-methylquinolinium cation and a 4-bromobenzenesulfonate anion (Fig. 1). The bond distances and angles in both the cation and anion are in normal ranges (Allen *et al.*, 1987) and are comparable to those in related structures (Jindawong *et al.*, 2005; Chantrapromma *et al.*, 2005, 2007). The cation is almost planar and exists in an *E* configuration. The dihedral angle between the quinolinium (C1–C9/N1) and the benzene ring of the cation is 5.1 (2)°. The methoxy group is coplanar with the attached ring, with a C19—O5—C14—C15 torsion angle of −179.1 (3)°.

In the crystal structure, atoms O1 and O3 of the anion are involved in weak C—H⋯O interactions, while atom O2 is involved in both weak C—H⋯O interactions and O—H⋯O

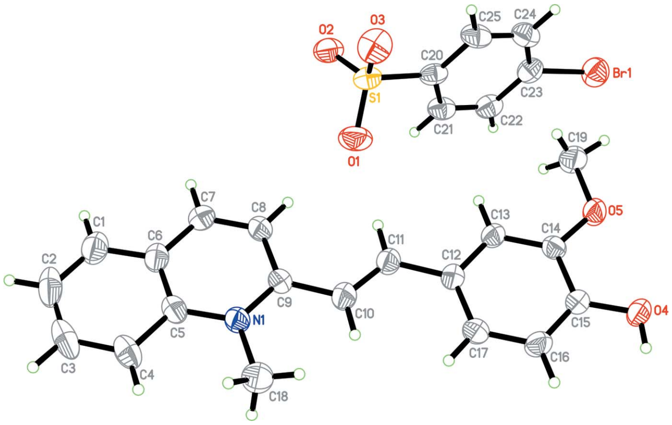


Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering scheme.

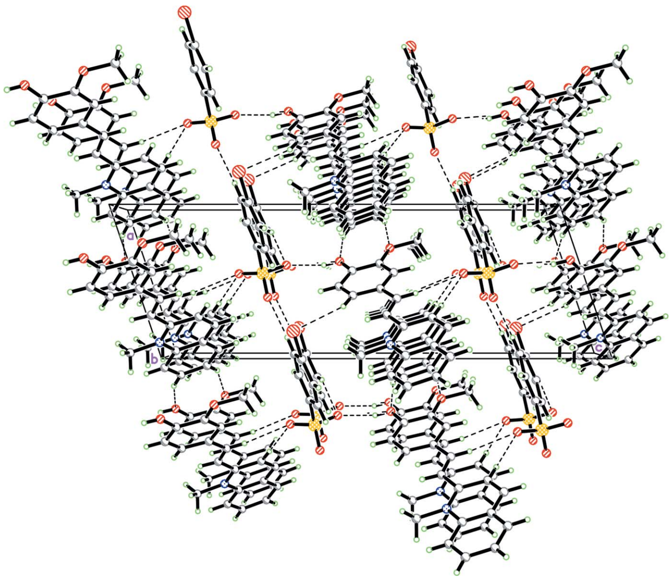


Figure 2
The crystal packing of (I), viewed down the *b* axis. Hydrogen bonds are shown as dashed lines.

hydrogen bonds (Table 2). The cations and anions form alternating layers parallel to the *ab* plane. These layers are interconnected through intermolecular O—H···O and C—H···O interactions, forming a three-dimensional network (Fig. 2 and Table 2).

Experimental

Compound (I) was synthesized by mixing solutions of silver(I) 4-bromobenzenesulfonate (0.20 g, 0.58 mmol) in hot methanol (55 ml) and 2-[(*E*)-2-(4-hydroxy-3-methoxyphenyl)ethenyl]-1-methylquinolinium iodide (0.28 g, 0.67 mmol) (Chantrapromma *et al.*, 2006) in hot methanol (150 ml). The mixing immediately yielded solid yellow silver iodide. The precipitate was removed by filtration and the red filtrate was evaporated under reduced pressure, yielding a dark-red solid (yield 0.28 g, 89%) which was recrystallized from methanol to give red–brown single crystal of compound (I) (m.p. 561–562 K).

Crystal data

$C_{19}H_{18}NO_2^+ \cdot C_6H_4BrO_3S^-$
M_r = 528.41
Monoclinic, *Pc*
a = 7.942 (3) Å
b = 6.751 (2) Å
c = 21.964 (8) Å
β = 108.861 (12)°
V = 1114.4 (7) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 1.98 mm^{-1}
T = 297 (2) K
0.56 × 0.31 × 0.05 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\rm min}$ = 0.403, $T_{\rm max}$ = 0.899
5986 measured reflections
4133 independent reflections
3711 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.032

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.090
S = 0.97
4133 reflections
304 parameters
5 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\rm max}$ = 0.60 e Å^{-3}
$\Delta\rho_{\rm min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), 1742 Friedel pairs
Flack parameter: 0.000 (7)

Table 1
Selected geometric parameters (Å, °).

Br1—C23	1.901 (4)	O5—C14	1.361 (4)
S1—O1	1.439 (3)	O5—C19	1.424 (4)
S1—O3	1.443 (3)	N1—C9	1.351 (4)
S1—O2	1.462 (3)	N1—C5	1.394 (4)
S1—C20	1.775 (4)	N1—C18	1.488 (4)
O4—C15	1.359 (4)	C10—C11	1.323 (5)
C9—C10—C11—C12	178.0 (4)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H1O4···O2$^{\rm i}$	0.81 (4)	1.88 (4)	2.677 (4)	166 (5)
C2—H2*A*···O5$^{\rm ii}$	0.93	2.48	3.337 (5)	154
C3—H3*A*···O4$^{\rm ii}$	0.93	2.55	3.409 (5)	153
C8—H8*A*···O1	0.93	2.42	3.347 (5)	177
C11—H11*A*···O1	0.93	2.47	3.400 (4)	173
C22—H22*A*···O3$^{\rm iii}$	0.93	2.28	3.204 (5)	177
C24—H24*A*···O2$^{\rm iv}$	0.93	2.48	3.269 (5)	142
C25—H25*A*···O3	0.93	2.56	2.919 (6)	103

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

The hydroxyl H atom was located in a difference map and refined isotropically. The remaining H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C) for aromatic, and C—H = 0.96 Å and $U_{\rm iso}$(H) = 1.5$U_{\rm eq}$(C) for methyl H atoms. A rotating-group model was used for the methyl 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

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to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

Financial support from the Center for Innovation in Chemistry: Postgraduate Education and Research Program in Chemistry (PERCH–CIC), Commission on Higher Education, Ministry of Education, Thailand, is gratefully acknowledged. The authors also thank Prince of Songkla University, the Malaysian Government and Universiti Sains Malaysia for Scientific Advancement Grant Allocation (SAGA) No. 304/PFIZIK/653003/A118.

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