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**Key indicators**Single-crystal X-ray study  
 $T = 100\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.004\text{ \AA}$   
 $R$  factor = 0.048  
 $wR$  factor = 0.112  
Data-to-parameter ratio = 21.4For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.**2-[(*E*)-2-(4-Methoxyphenyl)ethenyl]-1-methylquinolinium 4-bromobenzenesulfonate**

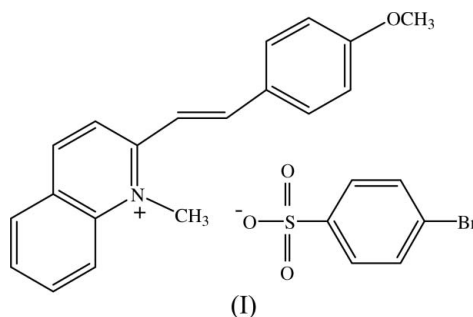
In the title compound  $\text{C}_{19}\text{H}_{18}\text{NO}^+\cdot\text{C}_6\text{H}_4\text{BrSO}_3^-$ , the cation is almost planar. The benzene ring of the anion makes dihedral angles of  $84.23(12)$  and  $84.59(15)^\circ$ , respectively, with the quinolinium group and the benzene ring of the cation. The cations and anions are arranged in an alternating one-dimensional chain along the  $b$  axis, and these chains are interconnected through  $\text{C}-\text{H}\cdots\text{O}$  and  $\text{C}-\text{H}\cdots\text{Br}$  interactions to form a three-dimensional network.  $\text{C}-\text{H}\cdots\pi$  interactions are also observed in the crystal structure.

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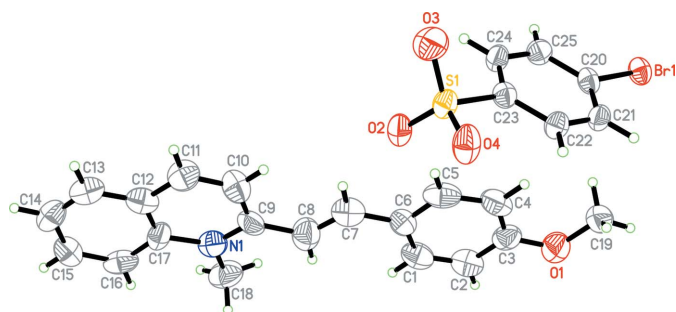
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**Comment**

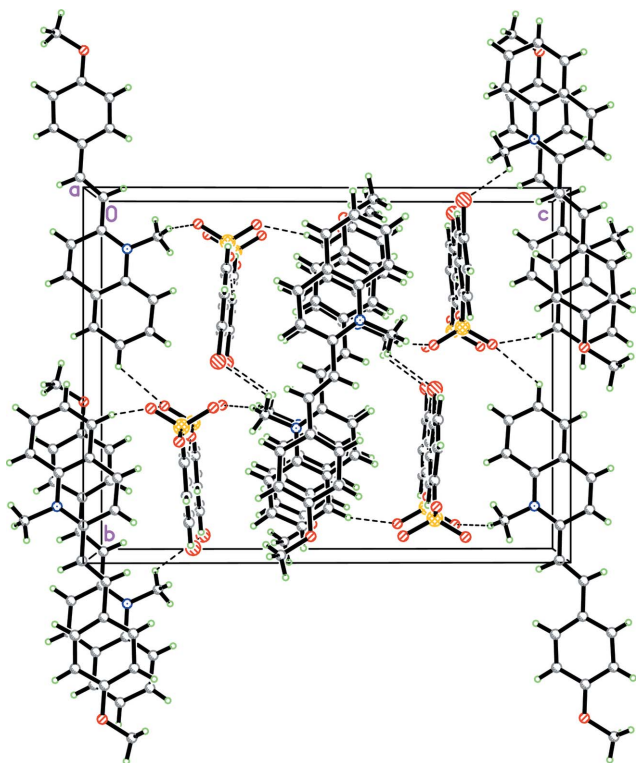
Our ongoing interest in new nonlinear optical (NLO) materials (Rahman *et al.*, 2003; Jindawong, Chantrapromma, Fun, Yu & Karalai, 2005; Jindawong, Chantrapromma, Fun & Karalai, 2005; Chantrapromma *et al.*, 2005, 2006) led us to synthesize the title compound, (I), in order to explore its molecular behaviour and crystal structure. However, since second-order nonlinear effects require a non-centrosymmetric structure for the bulk material (Williams, 1984) and (I) crystallizes in a centrosymmetric space group, it cannot exhibit second-order NLO properties.



The asymmetric unit of (I) consists of a  $\text{C}_{19}\text{H}_{18}\text{NO}^+$  cation and a  $\text{C}_6\text{H}_4\text{BrSO}_3^-$  anion (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-methylbenzenesulfonate, (II) (Jindawong, Chantrapromma, Fun & Karalai, 2005) and 2-[(*E*)-2-(3-hydroxy-4-methoxyphenyl)ethenyl]-1-methylquinolinium 4-chlorobenzenesulfonate, (III) (Chantrapromma *et al.*, 2006). In the cation, the quinolinium group (C9–C17/N1) is planar, with a maximum deviation from the plane of  $0.054(3)\text{ \AA}$  for atom N1. Overall, the cation is almost planar, as indicated by the dihedral angle of  $1.12(14)^\circ$  between the quinolinium group and the C1–C6 benzene ring. The H atoms attached to atoms C7 and C8 are mutually *trans*, so that the cation adopts an *E* configuration with a C6–C7–



**Figure 1**  
The asymmetric unit of (I), showing 80% probability displacement ellipsoids and the atomic numbering scheme.



**Figure 2**  
The crystal packing of (I), viewed down the *a* axis. Weak C—H...O and C—H...Br interactions are shown as dashed lines.

C8—C9 torsion angle of  $177.4(4)^\circ$ . The methoxy group deviates slightly from the plane of the benzene ring of the cation [C19—O1—C3—C4 =  $-5.6(5)^\circ$ ]. In the asymmetric unit, the molecular planes of the cation and anion are almost perpendicular to each other, with a dihedral angle of  $84.23(12)^\circ$  between the benzene ring of the anion and the quinolinium plane. This compares with  $59.17(9)^\circ$  in (II) and  $48.97(6)^\circ$  in (III). The angle between the benzene rings of the anion and cation is  $84.59(15)^\circ$  [ $60.59(10)^\circ$  in (II) and  $51.63(7)^\circ$  in (III)].

In the crystal structure, all the O atoms of the 4-bromobenzenesulfonate anion are involved in weak C—H...O interactions (Table 1 and Fig. 2). The cations and anions form alternating one-dimensional chains along the *b* axis. These chains are interconnected by weak C—H...O and C—H...Br interactions to form a three-dimensional molecular network.

C—H... $\pi$  interactions are also observed and details are given in Table 1.

## Experimental

Silver(I) 4-bromobenzenesulfonate (compound *A*) was synthesized as reported previously (Jindawong, Chantrapromma, Fun, Yu & Karalai, 2005). 2-(4'-Methoxystyryl)-1-methylquinolinium iodide (compound *B*) was synthesized by refluxing a solution of 1,2-dimethylquinolinium iodide (1.00 g, 3.51 mmol), 4-methoxybenzaldehyde (0.43 ml, 3.51 mmol) and piperidine (0.35 ml, 3.54 mmol), in a 1:1:1 molar ratio, in methanol (20 ml) for 7 h. The resulting solid was filtered off, washed with  $\text{CHCl}_3$  and recrystallized from  $\text{CH}_3\text{OH}$ , to give *B* as a green solid (0.95 g, 67%, mp. 498–499 K). The title compound, (I), was synthesized by mixing solutions of *A* (0.09 g, 0.25 mmol) and *B* (0.10 g, 0.25 mmol), each in hot MeOH (70 ml), which immediately gave a yellow mass of silver iodide. After stirring the mixture for 30 min, the silver iodide was removed and the resulting green–yellow solution was evaporated to yield a green–yellow solid. Single orange blocks of (I) were obtained by recrystallization from MeOH–EtOH (2:1 *v/v*) at ambient temperature over several days (m.p. 539–540 K).

### Crystal data

$\text{C}_{19}\text{H}_{18}\text{NO}^+ \cdot \text{C}_6\text{H}_4\text{BrO}_3\text{S}^-$   
 $M_r = 512.41$   
Monoclinic,  $P2_1/c$   
 $a = 7.1945(1) \text{ \AA}$   
 $b = 15.1542(2) \text{ \AA}$   
 $c = 19.6438(3) \text{ \AA}$   
 $\beta = 90.960(1)^\circ$   
 $V = 2141.40(5) \text{ \AA}^3$

$Z = 4$   
 $D_x = 1.589 \text{ Mg m}^{-3}$   
Mo  $K\alpha$  radiation  
 $\mu = 2.05 \text{ mm}^{-1}$   
 $T = 100.0(1) \text{ K}$   
Block, orange  
 $0.52 \times 0.37 \times 0.21 \text{ mm}$

### Data collection

Bruker SMART APEX2 CCD area-detector diffractometer  
 $\omega$  scans  
Absorption correction: multi-scan (SADABS; Bruker, 2005)  
 $T_{\min} = 0.415$ ,  $T_{\max} = 0.676$

25087 measured reflections  
6232 independent reflections  
4498 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.047$   
 $\theta_{\text{max}} = 30.0^\circ$

### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.048$   
 $wR(F^2) = 0.112$   
 $S = 1.05$   
6232 reflections  
291 parameters  
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 4.0824P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 1.38 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\text{min}} = -0.57 \text{ e \AA}^{-3}$

**Table 1**

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

Cg1 is the centroid of the C20–C25 ring.

D—H...A	D—H	H...A	D...A	D—H...A
C5—H5A...O2	0.93	2.54	3.436 (4)	162
C11—H11A...O4 <sup>i</sup>	0.93	2.58	3.481 (4)	162
C13—H13A...O3 <sup>i</sup>	0.93	2.52	3.382 (4)	155
C14—H14A...O3 <sup>ii</sup>	0.93	2.58	3.219 (4)	127
C18—H18C...O2 <sup>iii</sup>	0.96	2.32	3.252 (4)	165
C22—H22A...O4	0.93	2.54	2.919 (4)	105
C25—H25A...O4 <sup>iv</sup>	0.93	2.29	3.083 (4)	142
C4—H4A...Cg1	0.93	2.87	3.655 (4)	142

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

All H atoms bound to C atoms were refined using a riding model, with C–H = 0.93 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$  for aromatic H, and C–H = 0.96 Å and  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for CH<sub>3</sub> atoms. The highest peak is located 1.15 Å from H19C.

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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