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

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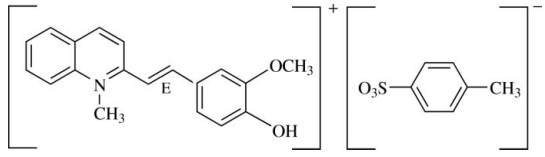
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.003 Å; R factor = 0.030; wR factor = 0.078; data-to-parameter ratio = 12.0.

In the title salt, $C_{19}H_{18}NO_2^+\cdot C_7H_7SO_3^-$, the C=C double bond in the cation has an E configuration. The cation is not planar as the dihedral angle between the quinolinium and benzene ring systems is 14.74 (8)°. The anion is aligned approximately perpendicularly to the cation, with the benzene ring of the anion making dihedral angles of 89.98 (8) and 75.36 (10)° with the quinolinium and benzene ring systems of the cation, respectively. An intramolecular O—H···O hydrogen bond between the hydroxy and methoxy groups generates an S(5) ring motif. The cations link with anions through weak C—H···O interaction into cation–anion pairs along the b direction, and the adjacent pairs are further linked by O—H···O hydrogen bonds and weak C—H···O interactions into a three-dimensional network. The crystal is further stabilized by C—H···π interactions, and π–π interactions [centroid–centroid distances of 3.5236 (12) and 3.5337 (12) Å] are also observed.

Related literature

For related structures, see, for example, Chantrapromma *et al.* (2006); Chantrapromma, Jindawong & Fun (2007); Chantrapromma, Jindawong, Fun & Patil (2007); Chantrapromma, Jindawong, Fun, Patil & Karalai (2007); Jindawong *et al.* (2005); Lakshmanaperumal *et al.* (2004). For literature on nonlinear optical activity, see Oudar & Chemla (1977); Williams (1984).



Experimental

Crystal data

$C_{19}H_{18}NO_2^+\cdot C_7H_7O_3S^-$
M_r = 463.53
Monoclinic, Pc
a = 6.9237 (5) Å
b = 11.1007 (7) Å
c = 15.1376 (9) Å
β = 106.507 (3)°
V = 1115.49 (13) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 297 (2) K
0.58 × 0.23 × 0.13 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.901, T_{max} = 0.976
5512 measured reflections
3665 independent reflections
3582 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.030
$wR(F^2)$ = 0.078
S = 1.07
3665 reflections
306 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Absolute structure: Flack (1983), 1698 Friedel pairs
Flack parameter: 0.03 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H1*O2*···O1	0.83 (3)	2.30 (3)	2.666 (2)	107 (2)
O2—H1*O2*···O5^{i}	0.83 (3)	1.89 (3)	2.655 (2)	154 (3)
C3—H3*A*···O4^{ii}	0.93	2.41	3.334 (3)	170
C5—H5*A*···O2^{iii}	0.93	2.39	3.149 (2)	139
C25—H25*A*···O3	0.93	2.51	2.897 (3)	106
C2—H2*A*···*Cg*4^{ii}	0.93	2.91	3.788 (2)	157
C7—H7*A*···*Cg*4	0.93	3.12	3.818 (2)	134
C8—H8*A*···*Cg*4	0.93	3.36	3.935 (2)	123
C13—H13*A*···*Cg*3^{iv}	0.93	3.24	3.556 (2)	102

Symmetry codes: (i) $x+1, y, z+1$; (ii) $x, y+1, z$; (iii) $x-1, y, z-1$; (iv) $x, -y+1, z+\frac{1}{2}$. *Cg*3 and *Cg*4 are centroids of the C1–C6 and C20–C25 benzene rings, respectively.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); 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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2386).

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supplementary materials

Acta Cryst. (2007). E**63**, o4928-o4929 [**doi:10.1107/S1600536807061922**]

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

S. Chantrapromma, B. Jindawong and H.-K. Fun

Comment

We have previously reported some crystal structures of quinolinium derivatives salts (Jindawong *et al.*, 2005; Chantrapromma *et al.*, 2006; Chantrapromma, Jindawong & Fun 2007; Chantrapromma, Jindawong, Fun & Patil, 2007; Chantrapromma, Jindawong, Fun, Patil & Karalai, 2007), which were synthesized to study for their nonlinear optic (NLO) properties. At molecular level, a generally popular approach towards NLO materials is systhesis of compounds of extended conjugated systems with donor and acceptor groups. Since compounds which are likely to exhibit large values of molecular hyperpolarizability (β) have to have polarizable electrons (conjugated π system) spread over a large distance (Oudar & Chemla, 1977), the title compound which is a benzene-based π-conjugated system was synthesized. The single-crystal *x*-ray structural study of the title compound was carried out in order to obtain detailed information on its crystal structure. The tile compound crystallized in the non-centrosymmetric monoclinic P*c* space group and therefore the title compound exhibits non-linear optical properties (Williams, 1984).

The asymmetric unit of the title compound consists of a $C_{19}H_{18}NO_2^+$ cation and a $C_7H_7SO_3^-$ anion (Fig. 1). The cation is not planar as indicated by the dihedral angle between the quinolinium and benzene rings being 14.74 (8) °. The H atoms attached to C10 and C11 are *trans* to each other; thus the cation exists in an *E* configuration [the C9–C10–C11–C12 torsion angle is −179.49 (18) °]. The structure of cation shows intramolecular O—H···O hydrogen bond between the hydroxy and methoxy groups which generates a S(5) ring motif (Bernstein *et al.*, 1995). The cation and anion are nearly perpendicular to each other which is indicated by the dihedral angles between the benzene ring of the 4-methylbenzenesulfonate anion with the quinolinium and benzene rings of the cation being 89.98 (8) ° and 75.36 (10) °, respectively.

In the crystal packing, O atoms of anion are involved in C—H···O weak interactions, (Table 1). The cations are linked with anions through weak C—H···O interaction [C3—H3A···O4; symmetry code *x*, 1 + *y*, *z*] (Table 1) into cation-anion pairs along the *b* direction and the adjacent pairs are further linked by O—H···O hydrogen bonds [O2—H1O2···O5; symmetry code 1 + *x*, *y*, 1 + *z*] and weak C—H···O interactions [C5—H5A···O2 symmetry code −1 + *x*, *y*, −1 + *z*] into a three dimension network. In addition, the cations are stacked along the *a* axis in such a way that the centroid–centroid distances between the N1/C1/C6–C9 ring (Cg_1) and C12–C17 ring (Cg_2) are 3.5236 (12) Å (symmetry code: *x*, 1 − *y*, −1/2 + *z*) and 3.5337 (12) Å (symmetry code: *x*, 1 − *y*, 1/2 + *z*), indicating π-π interactions. The crystal is further stabilized C—H···π interactions (Table 1); Cg_3 and Cg_4 are centroids of C1–C6 and C20–C25 benzene rings, respectively. Bond lengths and angles are in normal ranges and comparable with closely related structures (Chantrapromma, Jindawong & Fun, 2007; Chantrapromma, Jindawong, Fun & Patil, 2007; Chantrapromma, Jindawong, Fun, Patil & Karalai, 2007; Jindawong *et al.*, 2005; Lakshmanaperumal *et al.*, 2004).

Experimental

A 0.30 g (0.72 mmol) solution of 2-[(*E*)-2-(4-hydroxy-3-methoxy- phenyl)ethenyl]-1-methylquinolinium iodide (Chantrapromma *et al.*, 2007*b*) in hot methanol (150 ml) was mixed with 0.20 g (0.72 mmol) of silver (I) 4-methylben-

zenesulfonate in hot methanol (30 ml). The mixture turned to dark-red and cloudy immediately. After stirring for 30 min, the precipitate of silver iodide was filtered and the filtrate was evaporated to give a brown solid (0.31 g, 92%yield). Brown single crystals of the title compound suitable for X-ray structure determination were recrystallized from methanol after several days at ambient temperature. (Mp. 536–537 K).

Refinement

Hydroxy H atom was located in a difference map and isotropically refined. The remaining H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. The highest residual electron density peak is located at 0.93 Å from O4 and the deepest hole is located at 0.68 Å from S1.

Figures

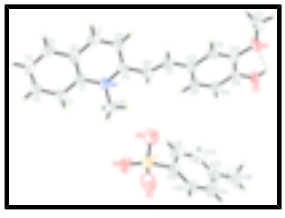


Fig. 1. The structure of (I) showing 50% probability displacement ellipsoids and the atom-numbering scheme. O—H···O hydrogen bond was drawn as a dash line.

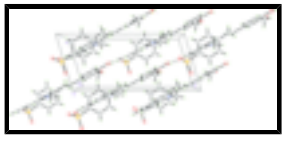


Fig. 2. The packing diagram of (I) viewd along the *a* axis. O—H···O hydrogen bonds and weak C—H···O interactions were drawn as dashed lines.

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

Crystal data

$C_{19}H_{18}NO_2^+ \cdot C_7H_7O_3S^-$	F_{000} = 488
M_r = 463.53	D_x = 1.380 Mg m^{-3}
Monoclinic, *Pc*	Melting point: 536-537 K
Hall symbol: P -2yc	Mo *K*α radiation λ = 0.71073 Å
a = 6.9237 (5) Å	Cell parameters from 3665 reflections
b = 11.1007 (7) Å	θ = 1.8–25.0º
c = 15.1376 (9) Å	μ = 0.18 mm^{-1}
β = 106.507 (3)º	*T* = 297 (2) K
V = 1115.49 (13) Å^3	Block, brown
Z = 2	0.58 × 0.23 × 0.13 mm

Data collection

Siemens SMART CCD area detector diffractometer	3665 independent reflections

Radiation source: medium-focus sealed tube	3582 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.014$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 25.0°$
$T = 297(2)$ K	$\theta_{min} = 1.8°$
ω scans	$h = -8 \rightarrow 8$
Absorption correction: empirical (using intensity measurements) (SADABS; Sheldrick, 1996)	$k = -9 \rightarrow 13$
$T_{min} = 0.901$, $T_{max} = 0.976$	$l = -17 \rightarrow 17$
5512 measured reflections	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.030$	$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.1204P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.078$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.07$	$\Delta\rho_{max} = 0.14$ e Å^{-3}
3665 reflections	$\Delta\rho_{min} = -0.17$ e Å^{-3}
306 parameters	Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
2 restraints	Extinction coefficient: 0.014 (2)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (Flack, 1983) parameter from 1698 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.03 (6)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.51215 (8)	0.16189 (4)	0.46563 (4)	0.04787 (14)
O1	1.3315 (2)	0.25370 (12)	1.22793 (10)	0.0551 (4)
O2	1.4831 (2)	0.45553 (14)	1.31606 (9)	0.0548 (4)
H1O2	1.488 (4)	0.389 (3)	1.341 (2)	0.075 (8)*

O3	0.3069 (2)	0.15382 (15)	0.46956 (12)	0.0705 (5)
O4	0.5685 (3)	0.06935 (13)	0.41122 (11)	0.0669 (5)
O5	0.5642 (3)	0.28182 (14)	0.44182 (11)	0.0699 (5)
N1	0.8616 (2)	0.68273 (13)	0.74870 (10)	0.0354 (3)
C1	0.7701 (2)	0.68972 (16)	0.65437 (12)	0.0348 (4)
C2	0.7145 (3)	0.80009 (17)	0.60887 (14)	0.0448 (4)
H2A	0.7363	0.8718	0.6420	0.054*
C3	0.6282 (3)	0.8017 (2)	0.51536 (15)	0.0538 (5)
H3A	0.5942	0.8751	0.4854	0.065*
C4	0.5903 (3)	0.6950 (2)	0.46436 (14)	0.0570 (6)
H4A	0.5294	0.6977	0.4012	0.068*
C5	0.6423 (3)	0.58759 (19)	0.50710 (13)	0.0478 (5)
H5A	0.6161	0.5168	0.4729	0.057*
C6	0.7353 (3)	0.58215 (16)	0.60236 (12)	0.0379 (4)
C7	0.8007 (3)	0.47260 (16)	0.64732 (13)	0.0433 (4)
H7A	0.7750	0.4007	0.6146	0.052*
C8	0.9009 (3)	0.47140 (17)	0.73804 (13)	0.0447 (4)
H8A	0.9499	0.3988	0.7663	0.054*
C9	0.9326 (3)	0.57791 (15)	0.79059 (13)	0.0386 (4)
C10	1.0436 (3)	0.57780 (17)	0.88764 (12)	0.0458 (4)
H10A	1.1008	0.6499	0.9137	0.055*
C11	1.0685 (3)	0.48202 (17)	0.94132 (12)	0.0424 (4)
H11A	1.0112	0.4105	0.9140	0.051*
C12	1.1766 (3)	0.47696 (16)	1.03886 (12)	0.0401 (4)
C13	1.1981 (3)	0.36561 (16)	1.08431 (13)	0.0401 (4)
H13A	1.1433	0.2968	1.0517	0.048*
C14	1.2991 (3)	0.35693 (16)	1.17639 (13)	0.0396 (4)
C15	1.3805 (3)	0.45985 (16)	1.22647 (12)	0.0395 (4)
C16	1.3588 (3)	0.56993 (17)	1.18148 (13)	0.0442 (4)
H16A	1.4127	0.6389	1.2142	0.053*
C17	1.2590 (3)	0.57861 (16)	1.08940 (13)	0.0427 (4)
H17A	1.2462	0.6533	1.0604	0.051*
C18	0.8755 (3)	0.79311 (18)	0.80513 (14)	0.0514 (5)
H18A	0.8529	0.7730	0.8631	0.077*
H18B	0.7756	0.8500	0.7731	0.077*
H18C	1.0071	0.8279	0.8158	0.077*
C19	1.2710 (4)	0.14166 (19)	1.18306 (17)	0.0551 (6)
H19A	1.3077	0.0775	1.2271	0.083*
H19B	1.3367	0.1303	1.1357	0.083*
H19C	1.1277	0.1416	1.1560	0.083*
C20	0.6664 (3)	0.14174 (15)	0.58113 (14)	0.0414 (4)
C21	0.8739 (3)	0.14691 (19)	0.60100 (17)	0.0559 (5)
H21A	0.9342	0.1568	0.5539	0.067*
C22	0.9915 (4)	0.1372 (2)	0.69183 (19)	0.0662 (7)
H22A	1.1309	0.1423	0.7048	0.079*
C23	0.9079 (4)	0.12039 (18)	0.76303 (16)	0.0612 (6)
C24	0.7022 (4)	0.1133 (2)	0.74191 (15)	0.0611 (6)
H24A	0.6420	0.1009	0.7888	0.073*
C25	0.5828 (3)	0.12419 (18)	0.65206 (14)	0.0488 (5)

H25A	0.4435	0.1195	0.6395	0.059*
C26	1.0397 (6)	0.1097 (3)	0.8620 (2)	0.0979 (10)
H26A	0.9599	0.0814	0.9003	0.147*
H26B	1.0953	0.1872	0.8835	0.147*
H26C	1.1470	0.0538	0.8648	0.147*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0664 (3)	0.0345 (2)	0.0378 (2)	0.0055 (2)	0.00683 (19)	0.0028 (2)
O1	0.0824 (10)	0.0344 (7)	0.0428 (8)	−0.0006 (6)	0.0085 (7)	0.0082 (6)
O2	0.0805 (10)	0.0435 (8)	0.0325 (7)	−0.0048 (7)	0.0031 (6)	0.0053 (6)
O3	0.0577 (10)	0.0778 (12)	0.0635 (10)	0.0028 (8)	−0.0028 (8)	−0.0065 (8)
O4	0.1095 (13)	0.0449 (8)	0.0466 (8)	0.0111 (8)	0.0226 (8)	0.0011 (7)
O5	0.1107 (14)	0.0400 (8)	0.0472 (8)	0.0014 (8)	0.0036 (8)	0.0130 (6)
N1	0.0400 (8)	0.0322 (7)	0.0329 (7)	0.0018 (6)	0.0085 (6)	−0.0010 (6)
C1	0.0334 (9)	0.0375 (9)	0.0330 (9)	0.0000 (7)	0.0087 (7)	−0.0003 (7)
C2	0.0540 (11)	0.0348 (9)	0.0436 (11)	0.0034 (8)	0.0105 (8)	0.0025 (8)
C3	0.0640 (14)	0.0507 (12)	0.0425 (11)	0.0050 (9)	0.0084 (9)	0.0127 (9)
C4	0.0638 (13)	0.0696 (14)	0.0312 (9)	0.0039 (10)	0.0031 (10)	0.0048 (9)
C5	0.0520 (12)	0.0528 (12)	0.0360 (10)	−0.0028 (9)	0.0084 (8)	−0.0076 (8)
C6	0.0384 (9)	0.0390 (9)	0.0360 (9)	−0.0015 (7)	0.0099 (8)	−0.0024 (7)
C7	0.0505 (11)	0.0319 (9)	0.0469 (11)	−0.0026 (8)	0.0131 (9)	−0.0069 (8)
C8	0.0537 (11)	0.0336 (9)	0.0435 (11)	0.0026 (8)	0.0086 (9)	0.0050 (7)
C9	0.0397 (9)	0.0368 (10)	0.0385 (9)	0.0004 (7)	0.0100 (8)	0.0038 (7)
C10	0.0540 (11)	0.0396 (10)	0.0385 (10)	−0.0020 (8)	0.0043 (8)	0.0028 (8)
C11	0.0446 (10)	0.0409 (10)	0.0394 (10)	−0.0013 (8)	0.0084 (8)	0.0012 (8)
C12	0.0415 (9)	0.0412 (10)	0.0385 (10)	0.0021 (8)	0.0125 (8)	0.0051 (8)
C13	0.0434 (10)	0.0373 (9)	0.0388 (9)	−0.0029 (7)	0.0103 (8)	0.0002 (7)
C14	0.0454 (10)	0.0348 (9)	0.0389 (9)	0.0027 (7)	0.0125 (8)	0.0058 (7)
C15	0.0437 (10)	0.0417 (10)	0.0331 (9)	0.0023 (7)	0.0110 (7)	0.0033 (7)
C16	0.0556 (12)	0.0347 (9)	0.0414 (10)	−0.0028 (8)	0.0122 (9)	0.0004 (7)
C17	0.0492 (10)	0.0389 (10)	0.0402 (10)	−0.0001 (8)	0.0129 (8)	0.0083 (8)
C18	0.0726 (14)	0.0388 (10)	0.0381 (10)	0.0047 (9)	0.0081 (9)	−0.0078 (8)
C19	0.0617 (13)	0.0368 (10)	0.0652 (15)	−0.0009 (9)	0.0158 (11)	0.0056 (9)
C20	0.0516 (11)	0.0288 (8)	0.0417 (10)	0.0040 (7)	0.0097 (8)	0.0044 (7)
C21	0.0552 (13)	0.0509 (12)	0.0642 (14)	0.0031 (9)	0.0212 (11)	0.0116 (10)
C22	0.0509 (13)	0.0510 (12)	0.0849 (18)	0.0051 (9)	0.0001 (12)	0.0059 (11)
C23	0.0856 (18)	0.0351 (10)	0.0506 (13)	0.0081 (10)	−0.0006 (11)	−0.0001 (9)
C24	0.0904 (18)	0.0496 (13)	0.0446 (11)	0.0080 (12)	0.0215 (12)	0.0033 (10)
C25	0.0569 (12)	0.0443 (11)	0.0459 (11)	0.0037 (9)	0.0160 (9)	0.0041 (9)
C26	0.135 (3)	0.0676 (17)	0.0595 (15)	0.0148 (17)	−0.0227 (16)	−0.0053 (14)

Geometric parameters (Å, °)

S1—O4	1.4383 (16)	C11—H11A	0.9300
S1—O3	1.4421 (19)	C12—C17	1.391 (3)
S1—O5	1.4511 (16)	C12—C13	1.402 (2)
S1—C20	1.785 (2)	C13—C14	1.374 (3)

O1—C14	1.369 (2)	C13—H13A	0.9300
O1—C19	1.422 (3)	C14—C15	1.398 (3)
O2—C15	1.341 (2)	C15—C16	1.386 (3)
O2—H1O2	0.83 (3)	C16—C17	1.372 (3)
N1—C9	1.349 (2)	C16—H16A	0.9300
N1—C1	1.390 (2)	C17—H17A	0.9300
N1—C18	1.481 (2)	C18—H18A	0.9600
C1—C2	1.405 (3)	C18—H18B	0.9600
C1—C6	1.413 (2)	C18—H18C	0.9600
C2—C3	1.371 (3)	C19—H19A	0.9600
C2—H2A	0.9300	C19—H19B	0.9600
C3—C4	1.397 (3)	C19—H19C	0.9600
C3—H3A	0.9300	C20—C25	1.371 (3)
C4—C5	1.356 (3)	C20—C21	1.383 (3)
C4—H4A	0.9300	C21—C22	1.389 (3)
C5—C6	1.404 (3)	C21—H21A	0.9300
C5—H5A	0.9300	C22—C23	1.374 (4)
C6—C7	1.404 (3)	C22—H22A	0.9300
C7—C8	1.351 (3)	C23—C24	1.370 (4)
C7—H7A	0.9300	C23—C26	1.522 (3)
C8—C9	1.407 (3)	C24—C25	1.382 (3)
C8—H8A	0.9300	C24—H24A	0.9300
C9—C10	1.452 (3)	C25—H25A	0.9300
C10—C11	1.319 (3)	C26—H26A	0.9600
C10—H10A	0.9300	C26—H26B	0.9600
C11—C12	1.454 (2)	C26—H26C	0.9600
O4—S1—O3	114.22 (10)	C12—C13—H13A	119.6
O4—S1—O5	112.71 (10)	O1—C14—C13	126.22 (17)
O3—S1—O5	112.61 (11)	O1—C14—C15	113.55 (15)
O4—S1—C20	106.70 (9)	C13—C14—C15	120.23 (16)
O3—S1—C20	105.91 (10)	O2—C15—C16	118.73 (17)
O5—S1—C20	103.68 (9)	O2—C15—C14	122.36 (16)
C14—O1—C19	118.80 (15)	C16—C15—C14	118.89 (16)
C15—O2—H1O2	116 (2)	C17—C16—C15	120.93 (17)
C9—N1—C1	121.99 (15)	C17—C16—H16A	119.5
C9—N1—C18	119.15 (14)	C15—C16—H16A	119.5
C1—N1—C18	118.83 (14)	C16—C17—C12	120.74 (17)
N1—C1—C2	122.27 (16)	C16—C17—H17A	119.6
N1—C1—C6	118.75 (15)	C12—C17—H17A	119.6
C2—C1—C6	118.97 (16)	N1—C18—H18A	109.5
C3—C2—C1	119.73 (19)	N1—C18—H18B	109.5
C3—C2—H2A	120.1	H18A—C18—H18B	109.5
C1—C2—H2A	120.1	N1—C18—H18C	109.5
C2—C3—C4	121.17 (19)	H18A—C18—H18C	109.5
C2—C3—H3A	119.4	H18B—C18—H18C	109.5
C4—C3—H3A	119.4	O1—C19—H19A	109.5
C5—C4—C3	119.95 (19)	O1—C19—H19B	109.5
C5—C4—H4A	120.0	H19A—C19—H19B	109.5
C3—C4—H4A	120.0	O1—C19—H19C	109.5

C4—C5—C6	120.67 (19)	H19A—C19—H19C	109.5
C4—C5—H5A	119.7	H19B—C19—H19C	109.5
C6—C5—H5A	119.7	C25—C20—C21	118.64 (19)
C5—C6—C7	121.72 (17)	C25—C20—S1	121.12 (15)
C5—C6—C1	119.47 (17)	C21—C20—S1	120.22 (16)
C7—C6—C1	118.78 (15)	C20—C21—C22	119.5 (2)
C8—C7—C6	120.19 (16)	C20—C21—H21A	120.2
C8—C7—H7A	119.9	C22—C21—H21A	120.2
C6—C7—H7A	119.9	C23—C22—C21	121.9 (2)
C7—C8—C9	121.25 (16)	C23—C22—H22A	119.1
C7—C8—H8A	119.4	C21—C22—H22A	119.1
C9—C8—H8A	119.4	C24—C23—C22	117.8 (2)
N1—C9—C8	118.79 (16)	C24—C23—C26	121.2 (3)
N1—C9—C10	119.58 (16)	C22—C23—C26	121.0 (3)
C8—C9—C10	121.61 (16)	C23—C24—C25	121.1 (2)
C11—C10—C9	124.26 (17)	C23—C24—H24A	119.5
C11—C10—H10A	117.9	C25—C24—H24A	119.5
C9—C10—H10A	117.9	C20—C25—C24	121.0 (2)
C10—C11—C12	126.58 (17)	C20—C25—H25A	119.5
C10—C11—H11A	116.7	C24—C25—H25A	119.5
C12—C11—H11A	116.7	C23—C26—H26A	109.5
C17—C12—C13	118.38 (16)	C23—C26—H26B	109.5
C17—C12—C11	122.63 (16)	H26A—C26—H26B	109.5
C13—C12—C11	118.99 (16)	C23—C26—H26C	109.5
C14—C13—C12	120.82 (17)	H26A—C26—H26C	109.5
C14—C13—H13A	119.6	H26B—C26—H26C	109.5
C9—N1—C1—C2	−173.31 (17)	C11—C12—C13—C14	179.98 (16)
C18—N1—C1—C2	8.7 (3)	C19—O1—C14—C13	5.3 (3)
C9—N1—C1—C6	5.5 (2)	C19—O1—C14—C15	−174.71 (18)
C18—N1—C1—C6	−172.56 (16)	C12—C13—C14—O1	−179.36 (19)
N1—C1—C2—C3	178.74 (18)	C12—C13—C14—C15	0.7 (3)
C6—C1—C2—C3	0.0 (3)	O1—C14—C15—O2	1.2 (3)
C1—C2—C3—C4	1.3 (3)	C13—C14—C15—O2	−178.87 (17)
C2—C3—C4—C5	−1.1 (3)	O1—C14—C15—C16	179.47 (17)
C3—C4—C5—C6	−0.3 (3)	C13—C14—C15—C16	−0.6 (3)
C4—C5—C6—C7	−176.40 (19)	O2—C15—C16—C17	178.55 (17)
C4—C5—C6—C1	1.6 (3)	C14—C15—C16—C17	0.2 (3)
N1—C1—C6—C5	179.77 (16)	C15—C16—C17—C12	0.1 (3)
C2—C1—C6—C5	−1.4 (3)	C13—C12—C17—C16	0.0 (3)
N1—C1—C6—C7	−2.2 (2)	C11—C12—C17—C16	179.62 (18)
C2—C1—C6—C7	176.66 (17)	O4—S1—C20—C25	−122.65 (17)
C5—C6—C7—C8	175.84 (18)	O3—S1—C20—C25	−0.58 (18)
C1—C6—C7—C8	−2.2 (3)	O5—S1—C20—C25	118.16 (16)
C6—C7—C8—C9	3.5 (3)	O4—S1—C20—C21	59.14 (17)
C1—N1—C9—C8	−4.3 (2)	O3—S1—C20—C21	−178.80 (16)
C18—N1—C9—C8	173.76 (18)	O5—S1—C20—C21	−60.06 (18)
C1—N1—C9—C10	174.23 (16)	C25—C20—C21—C22	−1.5 (3)
C18—N1—C9—C10	−7.8 (2)	S1—C20—C21—C22	176.71 (16)
C7—C8—C9—N1	−0.3 (3)	C20—C21—C22—C23	1.2 (3)

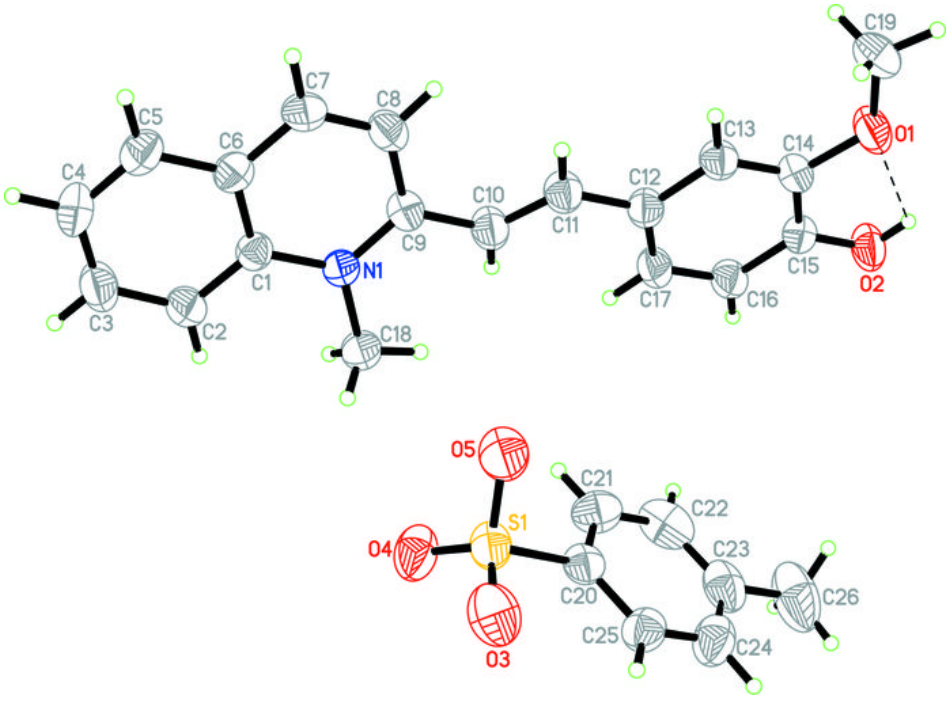
C7—C8—C9—C10	−178.76 (18)	C21—C22—C23—C24	0.0 (3)
N1—C9—C10—C11	159.44 (19)	C21—C22—C23—C26	179.8 (2)
C8—C9—C10—C11	−22.1 (3)	C22—C23—C24—C25	−0.8 (3)
C9—C10—C11—C12	−179.49 (18)	C26—C23—C24—C25	179.4 (2)
C10—C11—C12—C17	4.0 (3)	C21—C20—C25—C24	0.8 (3)
C10—C11—C12—C13	−176.44 (19)	S1—C20—C25—C24	−177.46 (16)
C17—C12—C13—C14	−0.4 (3)	C23—C24—C25—C20	0.4 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H1O2···O1	0.83 (3)	2.30 (3)	2.666 (2)	107 (2)
O2—H1O2···O5^{i}	0.83 (3)	1.89 (3)	2.655 (2)	154 (3)
C3—H3A···O4^{ii}	0.93	2.41	3.334 (3)	170
C5—H5A···O2^{iii}	0.93	2.39	3.149 (2)	139
C25—H25A···O3	0.93	2.51	2.897 (3)	106
C2—H2A···Cg4^{ii}	0.93	2.91	3.788 (2)	157
C7—H7A···Cg4	0.93	3.12	3.818 (2)	134
C8—H8A···Cg4	0.93	3.36	3.935 (2)	123
C13—H13A···Cg3^{iv}	0.93	3.24	3.556 (2)	102

Symmetry codes: (i) *x*+1, *y*, *z*+1; (ii) *x*, *y*+1, *z*; (iii) *x*−1, *y*, *z*−1; (iv) *x*, −*y*+1, *z*+1/2.

Fig. 1


C19
C7
C8
C5
C6
C13
C14
O1
C4
C12
C10
C11
C9
N1
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C15
O2
C3
C2
C17
C16
C18
O5
C21
C22
S1
O4
C23
C20
C26
C25
C24
O3

Fig. 2