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4-(4′-Hydroxy-3′-methoxystyryl)-1-methylpyridinium 0.58-bromide 0.42-iodide

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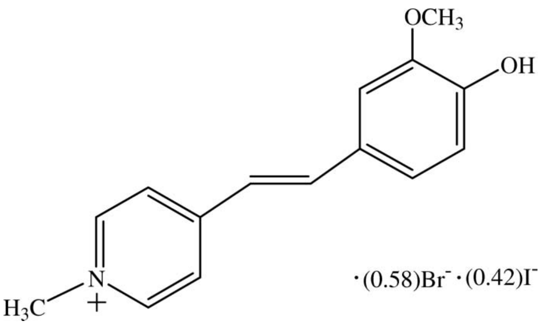
Key indicators: single-crystal X-ray study; T = 297 K; mean σ(C–C) = 0.005 Å; disorder in solvent or counterion; R factor = 0.072; wR factor = 0.216; data-to-parameter ratio = 13.9.

In the title compound, $C_{15}H_{16}NO_2^+\cdot 0.58Br^-\cdot 0.42I^-$, the cation is essentially planar, the dihedral angle between the two aromatic rings being 2.59 (18)°. The cations are linked into zigzag chains along the b axis by weak C—H⋯O hydrogen bonds, and the chains are linked to form a three-dimensional framework by O—H⋯Br, O—H⋯I (H⋯I = 1.97–2.48 Å) and C—H⋯I (H⋯I = 2.47–2.91 Å) hydrogen bonds, and π–π interactions involving the pyridinium and benzene rings [centroid–centroid distance is 3.518 (2) Å]. A single anion site is occupied at random by Br⁻ or I⁻.

Related literature

For bond-length data, see: Allen *et al.* (1987). For related structures, see: Jindawong *et al.* (2005); Chantrapromma *et al.* (2005); Chantrapromma, Ruanwas, Fun *et al.* (2006); Chantrapromma, Jindawong & Fun (2006); Chantrapromma, Ruanwas, Jindawong *et al.* (2006); Fun *et al.* (2006); Ruanwas *et al.* (2007); Chantrapromma *et al.* (2007); Patil *et al.* (2006); Shettigar *et al.* (2006).



Experimental

Crystal data

$C_{15}H_{16}NO_2^+\cdot 0.58Br^-\cdot 0.42I^-$
M_r = 341.93
Monoclinic, $P2_1/c$
a = 8.9627 (13) Å
b = 20.721 (3) Å
c = 8.0865 (12) Å
β = 103.304 (2)°
V = 1461.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 2.55 mm^{-1}
T = 297 (2) K
0.51 × 0.25 × 0.21 mm

Data collection

Siemens SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.458, $T_{\max}$ = 0.583
7691 measured reflections
2857 independent reflections
2417 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.072
$wR(F^2)$ = 0.216
S = 1.08
2857 reflections
206 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{\max}$ = 0.31 e Å^{-3}
$\Delta\rho_{\min}$ = −0.72 e Å^{-3}

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O1—H1O1⋯Br1	0.82	2.53	3.321 (3)	162
C12—H12⋯O1$^{\rm i}$	0.93	2.52	3.338 (5)	146

Symmetry code: (i) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

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: CI2384).

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supplementary materials

Acta Cryst. (2007). E**63**, o2882-o2883   [**doi:10.1107/S1600536807022076**]

4-(4'-Hydroxy-3'-methoxystyryl)-1-methylpyridinium 0.58-bromide 0.42-iodide

S. Chantrapromma and **H.-K. Fun**

Comment

In recent years, much effort has been focused on the development of new materials with non-linear optical (NLO) properties (Patil *et al.*, 2006; Shettigar *et al.*, 2006). In our continuing systamatic study of NLO materials (Jindawong *et al.*, 2005; Chantrapromma *et al.*, 2005; Chantrapromma, Ruanwas, Fun *et al.*, 2006; Chantrapromma, Jindawong & Fun, 2006; Chantrapromma, Ruanwas, Jindawong *et al.*, 2006; Fun *et al.*, 2006; Ruanwas *et al.*, 2007; Chantrapromma *et al.*, 2007), the title compound, (I), was synthesized and its crystal structure is reported here. Compound (I) crystallizes in a centrosymmetric space group and this precludes the presence of second-order NLO properties.

The refinement of (I) revealed the composition to be $C_{15}H_{16}NO_2^+.0.58Br^-.0.42I^-$ (Fig. 1), *i.e.* with fractional occupancy of the halide ions. Moreover, the iodide ion is disordered over three sites (I1A, I1B and I1C in Fig. 1). The cation exists in an *E* configuration with respect to the C7═C8 double bond [1.330 (6) Å], with the torsion angle C6–C7–C8–C9 being -178.8 (3)°. The bond lengths and angles (Table 1) have normal values (Allen *et al.*, 1987) and comparable to those in related structures (Jindawong *et al.*, 2005; Chantrapromma *et al.*, 2005; Chantrapromma, Ruanwas, Fun *et al.*, 2006; Chantrapromma, Jindawong & Fun, 2006; Chantrapromma, Ruanwas, Jindawong *et al.*, 2006; Ruanwas *et al.*, 2007; Chantrapromma *et al.*, 2007). The cation is essentially planar, the dihedral angle between the pyridinium and benzene rings is 2.59 (18)°. The C14—O2—C4—C5 torsion angle of -5.6 (6)° shows that the methoxy group is slightly twisted out of the benzene ring plane.

Intermolecular O—H···Br hydrogen bonds and weak C—H···O interactions are observed in the crystal structure of (I) (Table 1). The cations are linked together in a head-to-tail manner into zig-zag chains along the *b* axis through weak C—H···O interactions, and these chains are cross-linked by O—H···Br, O—H···I (H···I = 1.97-2.48 Å) and C—H···I (H···I = 2.47-2.91 Å) interactions forming a three-dimensional network (Fig. 2). The centroid-centroid distance between the N1/C9–C13 ring at (x, y, z) and the C1–C6 benzene ring at (2-x, -y, -1-z) is 3.518 (2) Å, indicating π-π interactions. A C12···I1A(-x, 1-y, 1-z) short contact [3.156 (7) Å] is observed in the crystal structure.

Experimental

Silver(I) 4-bromobenzenesulfonate (0.20 g, 0.59 mmol) in hot methanol (50 ml) was added to a solution of 4-(4'-hydroxy-3'-methoxystyryl)-1-methylpyridinium iodide (0.22 g, 0.59 mmol) in hot methanol (40 ml). The mixture immediately yielded a yellow solid of silver iodide which was filtered off after stirring the mixture for 30 min. The resulting red solution was evaporated to yield a red-brown solid. Brown block-shaped single crystals of (I) were obtained by recrystallization from methanol-ethanol (1:1 v/v) at room temperature after several days.

Refinement

The site occupancy factors for atoms Br1, I1A, I1B and I1C refined to 0.580 (3), 0.133 (2), 0.139 (2) and 0.148 (2), respectively. H atoms were placed in calculated positions, with O—H distance of 0.82 Å and C—H distances in the range 0.93–0.96 Å. The U_{iso} values were constrained to be $1.5U_{eq}$ of the carrier atom for hydroxyl and methyl H atoms and $1.2U_{eq}$ for the remaining H atoms. A rotating group model was used for the methyl groups. Owing to the large fraction of weak data at higher angles, the 2θ maximum was limited to 52°. The highest residual density peak is located 0.68 Å from atom C13 and the deepest hole is located 0.57 Å from atom Br1.

Figures

Fig. 1. The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

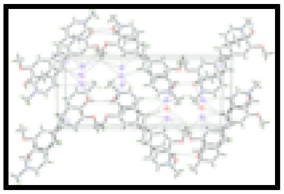

Fig. 2. The packing diagram of (I), viewed along the *c* axis. Hydrogen bonds are shown as dashed lines.

4-(4'-Hydroxy-3'-methoxystyryl)-1-methylpyridinium 0.58-bromide 0.42-iodide

Crystal data

$C_{15}H_{16}NO_2^{+}\cdot0.58Br^{-}\cdot0.42I^{-}$

$M_r = 341.93$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 8.9627\ (13)$ Å

$b = 20.721\ (3)$ Å

$c = 8.0865\ (12)$ Å

$\beta = 103.304\ (2)$°

$V = 1461.5\ (4)$ Å^3

$Z = 4$

$F_{000} = 686.2$

$D_x = 1.554$ Mg m^{-3}

Mo *K*α radiation
λ = 0.71073 Å

Cell parameters from 2857 reflections

θ = 2.0–26.0°

$\mu = 2.55$ mm^{-1}

$T = 297\ (2)$ K

Block, brown

0.51 × 0.25 × 0.21 mm

Data collection

Siemens SMART CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

Detector resolution: 8.33 pixels mm^{-1}

$T = 297(2)$ K

ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1996)

$T_{min} = 0.458$, $T_{max} = 0.583$

7691 measured reflections

2857 independent reflections

2417 reflections with $I > 2\sigma(I)$

$R_{int} = 0.024$

$\theta_{max} = 26.0$°

$\theta_{min} = 2.0$°

$h = -9 \rightarrow 11$

$k = -25 \rightarrow 19$

$l = -9 \rightarrow 9$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.072$

$wR(F^2) = 0.216$

$S = 1.08$

2857 reflections

206 parameters

1 restraint

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.1083P)^2 + 1.625P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.31$ e Å^{-3}

$\Delta\rho_{min} = -0.72$ e Å^{-3}

Extinction correction: none

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 > 2sigma(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}	Occ. (<1)
I1A	0.6170 (7)	0.6319 (3)	0.7668 (8)	0.155 (3)	0.133 (2)
I1B	0.7345 (9)	0.6386 (3)	0.5754 (7)	0.181 (3)	0.139 (2)
I1C	0.8589 (6)	0.6382 (3)	0.8253 (8)	0.169 (3)	0.148 (2)
Br1	0.72947 (12)	0.63747 (4)	0.73911 (13)	0.0761 (5)	0.580 (3)
O1	0.3913 (3)	0.68060 (15)	0.4999 (4)	0.0709 (9)	
H1O1	0.4627	0.6642	0.5691	0.106*	
O2	0.1697 (3)	0.71700 (14)	0.2545 (3)	0.0596 (7)	
N1	−0.4889 (3)	0.35571 (15)	−0.1165 (4)	0.0504 (7)	
C1	0.1803 (5)	0.5284 (2)	0.4242 (5)	0.0553 (9)	
H1	0.1863	0.4863	0.4651	0.066*	
C2	0.2924 (5)	0.5724 (2)	0.4963 (5)	0.0570 (9)	
H2	0.3728	0.5597	0.5850	0.068*	
C3	0.2858 (4)	0.63491 (19)	0.4377 (5)	0.0524 (9)	
C4	0.1610 (4)	0.65448 (18)	0.3036 (4)	0.0477 (8)	
C5	0.0524 (4)	0.61018 (19)	0.2341 (4)	0.0491 (8)	
H5	−0.0286	0.6228	0.1460	0.059*	

C6	0.0588 (4)	0.54602 (19)	0.2915 (4)	0.0495 (8)
C7	−0.0532 (4)	0.4967 (2)	0.2190 (5)	0.0537 (9)
H7	−0.0399	0.4564	0.2712	0.064*
C8	−0.1721 (4)	0.50257 (19)	0.0869 (5)	0.0520 (9)
H8	−0.1889	0.5426	0.0340	0.062*
C9	−0.2779 (4)	0.45054 (18)	0.0196 (4)	0.0480 (8)
C10	−0.4000 (4)	0.46270 (19)	−0.1185 (5)	0.0534 (9)
H10	−0.4120	0.5036	−0.1670	0.064*
C11	−0.5017 (4)	0.4153 (2)	−0.1830 (5)	0.0549 (9)
H11	−0.5821	0.4245	−0.2754	0.066*
C12	−0.3730 (4)	0.3415 (2)	0.0155 (5)	0.0555 (9)
H12	−0.3645	0.3001	0.0610	0.067*
C13	−0.2664 (4)	0.3878 (2)	0.0845 (5)	0.0542 (9)
H13	−0.1858	0.3771	0.1752	0.065*
C14	0.0455 (5)	0.7404 (2)	0.1262 (6)	0.0681 (11)
H14A	0.0667	0.7838	0.0969	0.102*
H14B	−0.0467	0.7398	0.1675	0.102*
H14C	0.0325	0.7134	0.0274	0.102*
C15	−0.6045 (6)	0.3056 (2)	−0.1849 (7)	0.0761 (13)
H15A	−0.5549	0.2693	−0.2228	0.114*
H15B	−0.6793	0.3231	−0.2788	0.114*
H15C	−0.6543	0.2921	−0.0976	0.114*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
I1A	0.109 (4)	0.178 (5)	0.180 (5)	0.002 (3)	0.034 (3)	0.028 (4)
I1B	0.219 (7)	0.194 (6)	0.120 (4)	0.030 (4)	0.020 (4)	0.007 (3)
I1C	0.126 (4)	0.189 (6)	0.171 (5)	−0.004 (3)	−0.010 (3)	0.020 (3)
Br1	0.0675 (7)	0.0599 (5)	0.0894 (7)	0.0047 (4)	−0.0053 (4)	0.0109 (4)
O1	0.0550 (17)	0.0665 (18)	0.078 (2)	−0.0038 (14)	−0.0127 (14)	−0.0072 (15)
O2	0.0544 (15)	0.0577 (16)	0.0601 (16)	−0.0027 (12)	−0.0003 (12)	0.0014 (12)
N1	0.0451 (16)	0.0563 (18)	0.0500 (17)	−0.0027 (13)	0.0113 (13)	−0.0026 (13)
C1	0.062 (2)	0.058 (2)	0.0466 (19)	−0.0003 (18)	0.0145 (16)	0.0046 (16)
C2	0.055 (2)	0.066 (2)	0.0457 (19)	0.0013 (18)	0.0042 (16)	0.0014 (17)
C3	0.0466 (19)	0.061 (2)	0.0462 (19)	−0.0006 (16)	0.0038 (15)	−0.0058 (16)
C4	0.0447 (18)	0.055 (2)	0.0432 (18)	0.0010 (15)	0.0092 (14)	−0.0044 (15)
C5	0.0424 (18)	0.064 (2)	0.0412 (17)	0.0029 (16)	0.0100 (14)	−0.0041 (15)
C6	0.0476 (18)	0.059 (2)	0.0452 (18)	−0.0052 (16)	0.0183 (15)	−0.0057 (15)
C7	0.053 (2)	0.059 (2)	0.053 (2)	−0.0001 (17)	0.0202 (16)	0.0015 (16)
C8	0.053 (2)	0.055 (2)	0.051 (2)	−0.0003 (16)	0.0182 (16)	0.0003 (16)
C9	0.0468 (18)	0.055 (2)	0.0464 (18)	0.0003 (15)	0.0185 (14)	−0.0044 (15)
C10	0.056 (2)	0.053 (2)	0.053 (2)	0.0045 (17)	0.0145 (16)	0.0008 (16)
C11	0.0475 (19)	0.066 (2)	0.050 (2)	0.0035 (17)	0.0082 (15)	−0.0028 (17)
C12	0.054 (2)	0.057 (2)	0.057 (2)	−0.0007 (17)	0.0155 (17)	0.0038 (17)
C13	0.0486 (19)	0.065 (2)	0.048 (2)	0.0043 (17)	0.0080 (15)	0.0018 (17)
C14	0.066 (3)	0.062 (2)	0.068 (3)	0.003 (2)	−0.001 (2)	0.006 (2)
C15	0.072 (3)	0.074 (3)	0.076 (3)	−0.023 (2)	0.003 (2)	−0.004 (2)

Geometric parameters (Å, °)

O1—C3	1.351 (5)	C7—H7	0.93
O1—H1O1	0.82	C8—C9	1.456 (5)
O2—C4	1.363 (5)	C8—H8	0.93
O2—C14	1.421 (5)	C9—C10	1.395 (5)
N1—C12	1.340 (5)	C9—C13	1.397 (5)
N1—C11	1.341 (5)	C10—C11	1.359 (6)
N1—C15	1.480 (5)	C10—H10	0.93
C1—C2	1.383 (6)	C11—H11	0.93
C1—C6	1.390 (5)	C12—C13	1.378 (6)
C1—H1	0.93	C12—H12	0.93
C2—C3	1.375 (6)	C13—H13	0.93
C2—H2	0.93	C14—H14A	0.96
C3—C4	1.426 (5)	C14—H14B	0.96
C4—C5	1.362 (5)	C14—H14C	0.96
C5—C6	1.405 (6)	C15—H15A	0.96
C5—H5	0.93	C15—H15B	0.96
C6—C7	1.458 (5)	C15—H15C	0.96
C7—C8	1.330 (6)		

C3—O1—H1O1	109.5	C9—C8—H8	117.8
C4—O2—C14	116.7 (3)	C10—C9—C13	116.4 (3)
C12—N1—C11	120.0 (3)	C10—C9—C8	119.3 (3)
C12—N1—C15	119.5 (4)	C13—C9—C8	124.3 (3)
C11—N1—C15	120.5 (4)	C11—C10—C9	120.7 (4)
C2—C1—C6	121.0 (4)	C11—C10—H10	119.7
C2—C1—H1	119.5	C9—C10—H10	119.7
C6—C1—H1	119.5	N1—C11—C10	121.6 (4)
C3—C2—C1	120.4 (4)	N1—C11—H11	119.2
C3—C2—H2	119.8	C10—C11—H11	119.2
C1—C2—H2	119.8	N1—C12—C13	120.6 (4)
O1—C3—C2	124.1 (4)	N1—C12—H12	119.7
O1—C3—C4	116.3 (3)	C13—C12—H12	119.7
C2—C3—C4	119.6 (3)	C12—C13—C9	120.7 (4)
C5—C4—O2	127.1 (3)	C12—C13—H13	119.6
C5—C4—C3	118.9 (4)	C9—C13—H13	119.6
O2—C4—C3	113.9 (3)	O2—C14—H14A	109.5
C4—C5—C6	122.0 (3)	O2—C14—H14B	109.5
C4—C5—H5	119.0	H14A—C14—H14B	109.5
C6—C5—H5	119.0	O2—C14—H14C	109.5
C1—C6—C5	118.0 (3)	H14A—C14—H14C	109.5
C1—C6—C7	118.1 (4)	H14B—C14—H14C	109.5
C5—C6—C7	123.9 (3)	N1—C15—H15A	109.5
C8—C7—C6	127.5 (4)	N1—C15—H15B	109.5
C8—C7—H7	116.2	H15A—C15—H15B	109.5
C6—C7—H7	116.2	N1—C15—H15C	109.5
C7—C8—C9	124.4 (4)	H15A—C15—H15C	109.5
C7—C8—H8	117.8	H15B—C15—H15C	109.5

C6—C1—C2—C3	0.0 (6)	C1—C6—C7—C8	−176.2 (4)
C1—C2—C3—O1	−179.3 (4)	C5—C6—C7—C8	3.1 (6)
C1—C2—C3—C4	1.0 (6)	C6—C7—C8—C9	178.8 (3)
C14—O2—C4—C5	5.7 (6)	C7—C8—C9—C10	179.2 (3)
C14—O2—C4—C3	−177.4 (3)	C7—C8—C9—C13	−0.7 (6)
O1—C3—C4—C5	179.0 (3)	C13—C9—C10—C11	0.7 (5)
C2—C3—C4—C5	−1.3 (5)	C8—C9—C10—C11	−179.2 (3)
O1—C3—C4—O2	1.8 (5)	C12—N1—C11—C10	−0.7 (6)
C2—C3—C4—O2	−178.5 (3)	C15—N1—C11—C10	177.7 (4)
O2—C4—C5—C6	177.4 (3)	C9—C10—C11—N1	0.2 (6)
C3—C4—C5—C6	0.5 (5)	C11—N1—C12—C13	0.1 (5)
C2—C1—C6—C5	−0.7 (5)	C15—N1—C12—C13	−178.2 (4)
C2—C1—C6—C7	178.6 (3)	N1—C12—C13—C9	0.8 (6)
C4—C5—C6—C1	0.4 (5)	C10—C9—C13—C12	−1.2 (5)
C4—C5—C6—C7	−178.8 (3)	C8—C9—C13—C12	178.7 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1O1···Br1	0.82	2.53	3.321 (3)	162
C12—H12···O1^{i}	0.93	2.52	3.338 (5)	146

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

Fig. 1

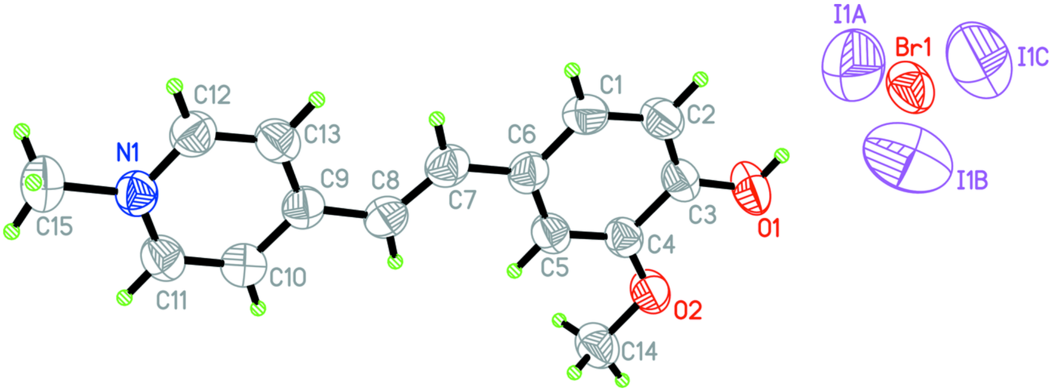
I1A
Br1
I1C
I1B
C12
C1
C2
C13
C6
N1
C9
C8
C7
C3
O1
C15
C4
C5
C10
C11
O2
C14

Fig. 2