Acta Crystallographica Section E
Structure Reports
Online
ISSN 1600-5368

(*S*)-(+)-1-(2-Bromophenyl)ethanol

Richard J. Staples*‡ and Jonathan W. Medley

Harvard University, Department of Chemistry and Chemical Biology, Cambridge, MA 02138, USA
Correspondence e-mail: staples@chemistry.msu.edu

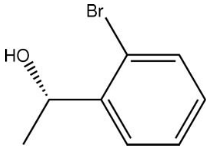
Received 26 October 2007; accepted 14 November 2007

Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.005 Å; R factor = 0.033; wR factor = 0.080; data-to-parameter ratio = 22.7.

The title compound, C_8H_9BrO, crystallizes with two molecules in the asymmetric unit. The structure displays O—H···O hydrogen bonding, generating zigzag chains evolving around a screw axis along [100].

Related literature

For literature on related complexes, see: Angiolini *et al.* (1995); Venkatachalam *et al.* (2005). For related literature, see: Staples (2001); Staples & George (2005); Staples & Huang (2002).



Experimental

Crystal data

C_8H_9BrO
M_r = 201.06
Orthorhombic, $P2_12_12_1$
a = 7.3235 (6) Å
b = 11.9440 (11) Å
c = 19.3583 (18) Å
V = 1693.3 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 4.79 mm^{-1}
T = 193 (2) K
0.20 × 0.08 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1998)
T_{min} = 0.434, T_{max} = 0.680
12365 measured reflections
4195 independent reflections
3420 reflections with $I > 2\sigma(I)$
R_{int} = 0.027

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.080
S = 1.03
4195 reflections
185 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.67 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}
Absolute structure: Flack (1983), with 1788 Friedel pairs
Flack parameter: −0.004 (10)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1*A*—H1*A*···O1*B*^{i}	0.84	1.81	2.645 (3)	177
O1*B*—H1*B*···O1*A*^{ii}	0.84	1.81	2.627 (3)	165

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 2003); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The CCD-based X-ray diffractometer at Harvard University was purchased through an NIH grant (1S10RR11937–01).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2123).

References

Angiolini, D., Geppi, M., Marchetti, F., Ruggeri, G. & Veracini, C. A. (1995). *Gazz. Chim. Ital.* **125**, 17–22.
Bruker (1997). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2000). *SHELXTL*. Version 6.14. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2003). *SAINT*. Version 6.25. Bruker AXS Inc., Madison, Wisconsin, USA.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1998). *SADABS*. University of Göttingen, Germany.
Staples, R. J. (2001). *Z. Kristallogr. New Cryst. Struct.* **216** , 311–312.
Staples, R. J. & George, S. (2005). *Z. Kristallogr. New Cryst. Struct.* **220**, 383–384.
Staples, R. J. & Huang, V. (2002). *Z. Kristallogr. New Cryst. Struct.* **217**, 554–555.
Venkatachalam, T. K., Zheng, Y., Ghosh, S. & Uckun, F. M. (2005). *J. Mol. Struct.* **743**, 103–115.

---

‡ Current address: Michigan State University, Department of Chemistry, East Lansing, MI 48824, USA.

doi:10.1107/S1600536807059260

supplementary materials

Acta Cryst. (2008). E**64**, o301 [**doi:10.1107/S1600536807059260**]

(*S*)-(+)-1-(2-Bromophenyl)ethanol

R. J. Staples and **J. W. Medley**

Comment

We have been studying the crystallization properties of enantiomeric compounds and their racemic mixtures, as well as the effect of hydrogen bonding on their crystallization behaviour (Staples and Huang, 2002; Staples and George, 2005). In particular we are interested in those compounds that can act as ligands to transition metal complexes (Staples, 2001). In the course of this study we have structurally characterized the tittle compound, C_8H_9BrO (I). We have also crystallized the enantiomeric compound, *R*-(-)-2-bromo-alpha-methyl benzylalcohol, which will be reported later.

S-(+)-2-bromo-alpha-methyl benzylalcohol crystallizes with two molecules in the assymmetric unit and presents intermolecular hydrogen bonding, a fact which can dictate the crystallization as well as solvation properties. It is our hope that we can use this compound for further studies of crystallization and coordination chemistry.

The stucture of *S*-(+)-2-bromo-alpha-methyl benzylalcohol is shown in Fgure 1. The compound exhibits standard bond lengths and angles, similar to those in closely related compounds (Angiolini *et al.*, 1995; Venkatachalam *et al.*,2005). It displays hydrogen bonding interactions with neighboring molecules (Table 1), to form a linear type of hydrogen bonding structure (Figure 2). The outcome is a zigzag chain structure containing both unique molecules and evolving around a screw axis along [100].

Experimental

The title compound was purchased from Aldrich and the crystals were grown by a slow evaporation of a dichloromethane solution.

Refinement

All H atoms were found by difference Fourier methods and refined isotropically.

Figures

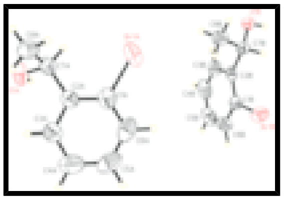


Fig. 1. Thermal ellipsoid plot (50% probability) of the title compound.

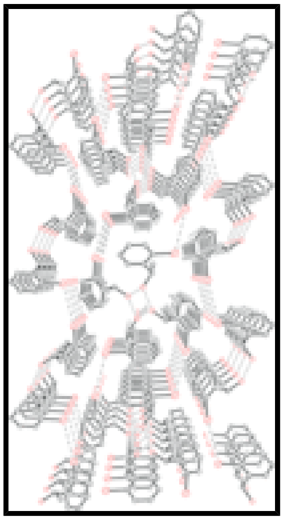


Fig. 2. Packing diagram of the title compund showing the linear hydrogen bonding interaction.

(*S*)-(+)-1-(2-Bromophenyl)ethanol

Crystal data

C_8H_9BrO

M_r = 201.06

Orthorhombic, $P2_12_12_1$

Hall symbol: P 2ac 2ab

a = 7.3235 (6) Å

b = 11.9440 (11) Å

c = 19.3583 (18) Å

V = 1693.3 (3) Å^3

Z = 8

F_{000} = 800

D_x = 1.577 Mg m^{-3}

Mo $K\alpha$ radiation
λ = 0.71073 Å

Cell parameters from 3839 reflections

θ = 3.0–23.9°

μ = 4.79 mm^{-1}

T = 193 (2) K

Needle, white

0.20 × 0.08 × 0.08 mm

Data collection

Bruker SMART CCD area-detector diffractometer

Radiation source: normal-focus sealed tube

Monochromator: graphite

T = 193(2) K

phi and ω scans

Absorption correction: multi-scan (SADABS; Sheldrick, 1998)

$T_{\min}$ = 0.434, $T_{\max}$ = 0.680

12365 measured reflections

4195 independent reflections

3420 reflections with $I > 2\sigma(I)$

$R_{\rm int}$ = 0.027

$\theta_{\max}$ = 28.3°

$\theta_{\min}$ = 2.0°

$h = -7\rightarrow9$

$k = -15\rightarrow12$

$l = -25\rightarrow21$

Refinement

Refinement on F^2

Least-squares matrix: full

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.0359P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.080$	$(\Delta/\sigma)_{max} = 0.001$
$S = 1.03$	$\Delta\rho_{max} = 0.67$ e Å^{-3}
4195 reflections	$\Delta\rho_{min} = -0.32$ e Å^{-3}
185 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack, 1983, 1788 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: −0.004 (10)

Special details

Experimental. Data was collected using a BRUKER *SMART* CCD (charge coupled device) based diffractometer equipped with an Oxford low-temperature apparatus operating at 193 K. A suitable crystal was chosen and mounted on a glass fiber using grease. Data were measured using omega scans of 0.3° per frame for 30 s, such that a hemisphere was collected. A total of 1271 frames were collected with a final resolution of 0.76 Å. The first 50 frames were recollected at the end of data collection to monitor for decay. Cell parameters were retrieved using *SMART* software and refined using *SAINT* on all observed reflections. Data reduction was performed using the *SAINT* software which corrects for Lp and decay. The structures are solved by the direct method using the *SHELX90* program and refined by least squares method on F2 *SHELXL93*, incorporated in *SHELXTL* V6.1.

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 $F^2 > 2\text{sigma}(F^2)$ 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}
Br1A	0.13612 (6)	0.57908 (3)	0.20047 (2)	0.07072 (14)
O1A	0.0096 (3)	0.29862 (17)	0.05433 (10)	0.0494 (5)
H1A	0.1035	0.3182	0.0326	0.074*
C1A	0.2226 (4)	0.4285 (2)	0.20561 (15)	0.0458 (7)
C2A	0.1479 (4)	0.3466 (2)	0.16427 (14)	0.0403 (6)
C3A	0.2190 (5)	0.2392 (3)	0.17111 (16)	0.0553 (8)
H3A	0.1718	0.1807	0.1431	0.066*
C4A	0.3564 (5)	0.2154 (4)	0.2175 (2)	0.0701 (10)
H4A	0.4020	0.1413	0.2217	0.084*
C5A	0.4272 (5)	0.3004 (4)	0.25806 (19)	0.0675 (10)
H5A	0.5222	0.2843	0.2900	0.081*
C6A	0.3622 (4)	0.4066 (3)	0.25272 (17)	0.0606 (9)
H6A	0.4110	0.4649	0.2806	0.073*
C7A	−0.0089 (4)	0.3657 (2)	0.11472 (14)	0.0414 (6)
H7A	−0.0110	0.4464	0.1010	0.050*

C8A	−0.1898 (4)	0.3363 (3)	0.14870 (16)	0.0518 (7)
H8A1	−0.2888	0.3447	0.1151	0.078*
H8A2	−0.2112	0.3864	0.1879	0.078*
H8A3	−0.1859	0.2586	0.1650	0.078*
Br1B	1.09635 (5)	0.88973 (3)	0.153281 (17)	0.06112 (12)
O1B	0.8026 (3)	1.13185 (16)	0.01304 (11)	0.0500 (5)
H1B	0.8822	1.1806	0.0214	0.075*
C1B	1.1100 (4)	0.8977 (2)	0.05449 (14)	0.0407 (6)
C2B	0.9897 (4)	0.9647 (2)	0.01929 (14)	0.0380 (6)
C3B	1.0055 (5)	0.9659 (3)	−0.05293 (15)	0.0493 (7)
H3B	0.9253	1.0111	−0.0796	0.059*
C4B	1.1372 (5)	0.9016 (3)	−0.08555 (18)	0.0623 (9)
H4B	1.1466	0.9031	−0.1345	0.075*
C5B	1.2543 (5)	0.8358 (3)	−0.0479 (2)	0.0618 (9)
H5B	1.3445	0.7924	−0.0709	0.074*
C6B	1.2412 (4)	0.8325 (3)	0.02258 (19)	0.0525 (8)
H6B	1.3206	0.7865	0.0490	0.063*
C7B	0.8394 (4)	1.0340 (2)	0.05289 (14)	0.0405 (6)
H7B	0.8787	1.0565	0.1004	0.049*
C8B	0.6624 (4)	0.9675 (3)	0.05759 (18)	0.0536 (8)
H8B1	0.5701	1.0119	0.0820	0.080*
H8B2	0.6844	0.8976	0.0828	0.080*
H8B3	0.6186	0.9501	0.0110	0.080*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1A	0.0939 (3)	0.04272 (17)	0.0756 (2)	−0.00522 (18)	0.0009 (2)	−0.01741 (16)
O1A	0.0535 (13)	0.0491 (11)	0.0457 (11)	−0.0190 (10)	0.0097 (9)	−0.0088 (9)
C1A	0.0491 (17)	0.0454 (15)	0.0431 (15)	−0.0093 (13)	0.0102 (13)	0.0011 (13)
C2A	0.0390 (14)	0.0387 (13)	0.0433 (15)	−0.0040 (12)	0.0092 (11)	0.0043 (11)
C3A	0.0552 (19)	0.0476 (18)	0.063 (2)	0.0002 (15)	−0.0012 (15)	0.0025 (14)
C4A	0.055 (2)	0.071 (2)	0.084 (2)	0.0115 (18)	0.0002 (19)	0.021 (2)
C5A	0.0398 (19)	0.095 (3)	0.068 (2)	−0.0068 (19)	−0.0046 (16)	0.023 (2)
C6A	0.050 (2)	0.079 (3)	0.0525 (18)	−0.0225 (19)	−0.0002 (14)	0.0029 (16)
C7A	0.0470 (16)	0.0328 (13)	0.0443 (15)	−0.0035 (12)	0.0025 (12)	0.0024 (11)
C8A	0.0457 (16)	0.0612 (19)	0.0484 (16)	0.0059 (14)	0.0041 (14)	0.0050 (15)
Br1B	0.0701 (2)	0.0615 (2)	0.05172 (18)	0.01563 (17)	−0.01687 (16)	0.00621 (14)
O1B	0.0485 (11)	0.0327 (10)	0.0688 (13)	−0.0017 (9)	−0.0228 (10)	0.0000 (9)
C1B	0.0397 (14)	0.0333 (13)	0.0492 (14)	−0.0042 (12)	−0.0054 (11)	0.0005 (11)
C2B	0.0382 (14)	0.0275 (12)	0.0483 (16)	−0.0059 (11)	−0.0018 (12)	−0.0021 (11)
C3B	0.0575 (19)	0.0418 (15)	0.0484 (17)	−0.0085 (15)	−0.0027 (14)	0.0026 (12)
C4B	0.074 (2)	0.056 (2)	0.0568 (18)	−0.0197 (19)	0.0196 (16)	−0.0120 (15)
C5B	0.057 (2)	0.0431 (17)	0.085 (3)	−0.0043 (17)	0.0241 (19)	−0.0118 (17)
C6B	0.0377 (16)	0.0399 (16)	0.080 (2)	0.0003 (13)	0.0012 (15)	−0.0017 (15)
C7B	0.0416 (15)	0.0359 (13)	0.0440 (15)	0.0019 (13)	−0.0105 (12)	0.0015 (11)
C8B	0.0430 (17)	0.0472 (16)	0.071 (2)	0.0004 (15)	0.0005 (15)	0.0032 (15)

Geometric parameters (Å, °)

Br1A—C1A	1.909 (3)	Br1B—C1B	1.917 (3)
O1A—C7A	1.424 (3)	O1B—C7B	1.426 (3)
O1A—H1A	0.8400	O1B—H1B	0.8400
C1A—C2A	1.378 (4)	C1B—C2B	1.370 (4)
C1A—C6A	1.395 (4)	C1B—C6B	1.383 (4)
C2A—C3A	1.391 (4)	C2B—C3B	1.403 (4)
C2A—C7A	1.514 (4)	C2B—C7B	1.523 (4)
C3A—C4A	1.378 (5)	C3B—C4B	1.385 (5)
C3A—H3A	0.9500	C3B—H3B	0.9500
C4A—C5A	1.384 (6)	C4B—C5B	1.373 (5)
C4A—H4A	0.9500	C4B—H4B	0.9500
C5A—C6A	1.359 (6)	C5B—C6B	1.369 (5)
C5A—H5A	0.9500	C5B—H5B	0.9500
C6A—H6A	0.9500	C6B—H6B	0.9500
C7A—C8A	1.520 (4)	C7B—C8B	1.523 (4)
C7A—H7A	1.0000	C7B—H7B	1.0000
C8A—H8A1	0.9800	C8B—H8B1	0.9800
C8A—H8A2	0.9800	C8B—H8B2	0.9800
C8A—H8A3	0.9800	C8B—H8B3	0.9800

C7A—O1A—H1A	109.5	C7B—O1B—H1B	109.5
C2A—C1A—C6A	122.5 (3)	C2B—C1B—C6B	123.6 (3)
C2A—C1A—Br1A	120.5 (2)	C2B—C1B—Br1B	119.4 (2)
C6A—C1A—Br1A	117.0 (2)	C6B—C1B—Br1B	117.0 (2)
C1A—C2A—C3A	116.8 (3)	C1B—C2B—C3B	116.7 (3)
C1A—C2A—C7A	124.2 (3)	C1B—C2B—C7B	124.7 (3)
C3A—C2A—C7A	118.9 (3)	C3B—C2B—C7B	118.6 (3)
C4A—C3A—C2A	121.7 (3)	C4B—C3B—C2B	120.4 (3)
C4A—C3A—H3A	119.2	C4B—C3B—H3B	119.8
C2A—C3A—H3A	119.2	C2B—C3B—H3B	119.8
C3A—C4A—C5A	119.5 (4)	C5B—C4B—C3B	120.7 (3)
C3A—C4A—H4A	120.3	C5B—C4B—H4B	119.6
C5A—C4A—H4A	120.3	C3B—C4B—H4B	119.6
C6A—C5A—C4A	120.7 (3)	C6B—C5B—C4B	120.1 (3)
C6A—C5A—H5A	119.6	C6B—C5B—H5B	120.0
C4A—C5A—H5A	119.6	C4B—C5B—H5B	120.0
C5A—C6A—C1A	118.8 (3)	C5B—C6B—C1B	118.5 (3)
C5A—C6A—H6A	120.6	C5B—C6B—H6B	120.7
C1A—C6A—H6A	120.6	C1B—C6B—H6B	120.7
O1A—C7A—C2A	111.3 (2)	O1B—C7B—C8B	107.4 (2)
O1A—C7A—C8A	107.9 (2)	O1B—C7B—C2B	110.6 (2)
C2A—C7A—C8A	110.6 (2)	C8B—C7B—C2B	110.9 (2)
O1A—C7A—H7A	109.0	O1B—C7B—H7B	109.3
C2A—C7A—H7A	109.0	C8B—C7B—H7B	109.3
C8A—C7A—H7A	109.0	C2B—C7B—H7B	109.3
C7A—C8A—H8A1	109.5	C7B—C8B—H8B1	109.5
C7A—C8A—H8A2	109.5	C7B—C8B—H8B2	109.5

H8A1—C8A—H8A2	109.5	H8B1—C8B—H8B2	109.5
C7A—C8A—H8A3	109.5	C7B—C8B—H8B3	109.5
H8A1—C8A—H8A3	109.5	H8B1—C8B—H8B3	109.5
H8A2—C8A—H8A3	109.5	H8B2—C8B—H8B3	109.5
C6A—C1A—C2A—C3A	−0.4 (4)	C6B—C1B—C2B—C3B	−0.6 (4)
Br1A—C1A—C2A—C3A	179.8 (2)	Br1B—C1B—C2B—C3B	−179.3 (2)
C6A—C1A—C2A—C7A	177.3 (3)	C6B—C1B—C2B—C7B	177.6 (3)
Br1A—C1A—C2A—C7A	−2.5 (4)	Br1B—C1B—C2B—C7B	−1.1 (4)
C1A—C2A—C3A—C4A	0.7 (4)	C1B—C2B—C3B—C4B	0.1 (4)
C7A—C2A—C3A—C4A	−177.1 (3)	C7B—C2B—C3B—C4B	−178.2 (3)
C2A—C3A—C4A—C5A	−0.7 (5)	C2B—C3B—C4B—C5B	0.0 (5)
C3A—C4A—C5A—C6A	0.3 (6)	C3B—C4B—C5B—C6B	0.4 (5)
C4A—C5A—C6A—C1A	0.0 (5)	C4B—C5B—C6B—C1B	−0.8 (5)
C2A—C1A—C6A—C5A	0.0 (5)	C2B—C1B—C6B—C5B	1.0 (4)
Br1A—C1A—C6A—C5A	179.8 (3)	Br1B—C1B—C6B—C5B	179.7 (2)
C1A—C2A—C7A—O1A	145.5 (3)	C1B—C2B—C7B—O1B	150.2 (2)
C3A—C2A—C7A—O1A	−36.9 (3)	C3B—C2B—C7B—O1B	−31.6 (3)
C1A—C2A—C7A—C8A	−94.5 (3)	C1B—C2B—C7B—C8B	−90.7 (3)
C3A—C2A—C7A—C8A	83.1 (3)	C3B—C2B—C7B—C8B	87.5 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1A—H1A···O1B^{i}	0.84	1.81	2.645 (3)	177
O1B—H1B···O1A^{ii}	0.84	1.81	2.627 (3)	165

Symmetry codes: (i) *x*−1/2, −*y*+3/2, −*z*; (ii) *x*+1, *y*+1, *z*.

Fig. 1

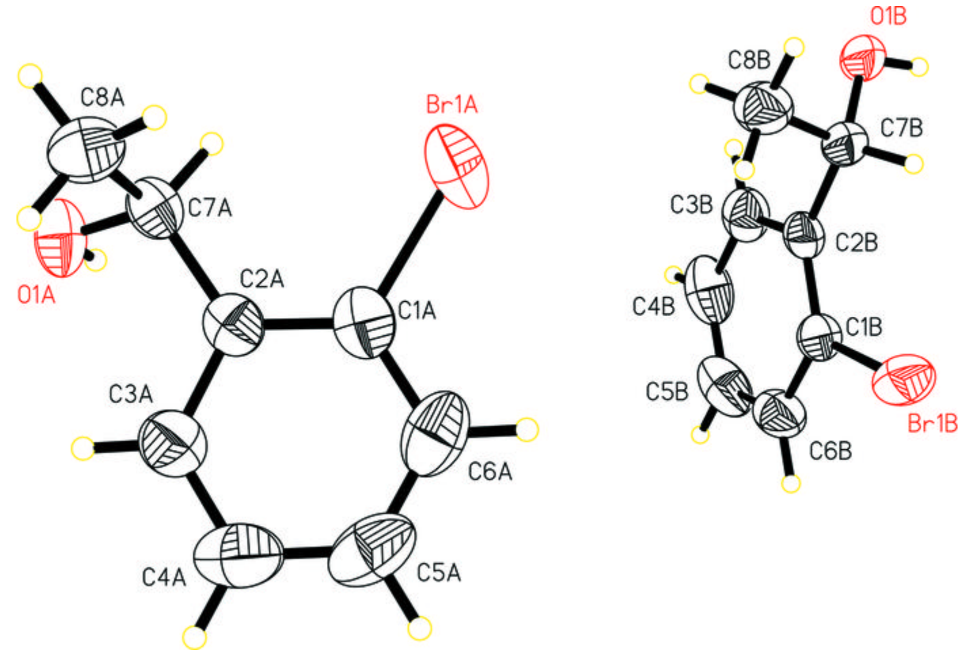

C8A
Br1A
C7A
O1A
C2A
C1A
C3A
C6A
C4A
C5A
O1B
C8B
C7B
C3B
C2B
C4B
C1B
C5B
Br1B
C6B

Fig. 2