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(E)-1-(2-Bromophenyl)-3-(2,5-dimethoxyphenyl)prop-2-en-1-one

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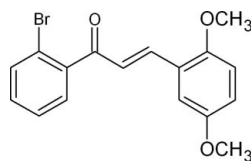
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Key indicators: single-crystal X-ray study; $T = 110$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.053; wR factor = 0.146; data-to-parameter ratio = 14.8.

The title compound, $\text{C}_{17}\text{H}_{15}\text{BrO}_3$, is a chalcone with the 2-bromophenyl and 2,5-dimethoxyphenyl rings bonded at opposite ends of a propene group. The dihedral angle between the mean planes of the *ortho*-bromo and *ortho,meta*-dimethoxy-substituted benzene rings is 77.3 (1)°. The dihedral angles between the mean plane of the prop-2-ene-1-one group and the mean planes of the 2-bromophenyl and 2,5-dimethoxyphenyl rings are 58.6 (1) and 30.7 (4)°, respectively. Weak $\text{C}-\text{H}\cdots\text{O}$, $\text{C}-\text{H}\cdots\text{Br}$ and $\pi-\pi$ stacking intermolecular interactions [centroid-centroid distance = 3.650 (2) Å] are present in the structure.

Related literature

For the radical quenching properties of included phenol groups, see: Dhar (1981). For their anticancer activity, see Dimmock *et al.* (1999). For related structures, see: Ng *et al.* (2006); Rosli *et al.* (2006). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{15}\text{BrO}_3$
 $M_r = 347.20$

Triclinic, $P\bar{1}$
 $a = 7.7643$ (9) Å

$b = 9.7006$ (11) Å
 $c = 10.2722$ (10) Å
 $\alpha = 72.901$ (10)°
 $\beta = 78.487$ (9)°
 $\gamma = 86.359$ (9)°
 $V = 724.59$ (14) Å³

$Z = 2$
Cu $K\alpha$ radiation
 $\mu = 3.93$ mm⁻¹
 $T = 110$ K
 $0.54 \times 0.26 \times 0.08$ mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2007)
 $T_{\min} = 0.179$, $T_{\max} = 0.635$

4759 measured reflections
2835 independent reflections
2749 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$
 $wR(F^2) = 0.146$
 $S = 1.05$
2835 reflections

192 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 2.51$ e Å⁻³
 $\Delta\rho_{\text{min}} = -1.11$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{C4}-\text{H4}\cdots\text{Br1}^i$	0.95	2.95	3.834 (4)	155
$\text{C3}-\text{H3}\cdots\text{O2}^{ii}$	0.95	2.62	3.463 (5)	148

Symmetry codes: (i) $x + 1, y, z$; (ii) $-x + 1, -y + 2, -z$.

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2007); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FB2201).

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supplementary materials

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(E)-1-(2-Bromophenyl)-3-(2,5-dimethoxyphenyl)prop-2-en-1-one

J. P. Jasinski, R. J. Butcher, K. Veena, B. Narayana and H. S. Yathirajan

Comment

Chalcones, or 1,3-diaryl-2-propen-1-ones, belong to the flavonoid family. Chemically they consist of open-chain flavonoids in which the two aromatic rings are joined by a three-carbon α,β -unsaturated carbonyl system. A vast number of naturally occurring chalcones are polyhydroxylated in the aryl rings. The radical quenching properties of the phenol groups present in many chalcones have raised interest in using the compounds or chalcone rich plant extracts as drugs or food preservatives (Dhar, 1981). Chalcones have been reported to possess many useful biological properties, including anti-inflammatory, antimicrobial, antifungal, antioxidant, cytotoxic, anticancer activities (Dimmock *et al.*, 1999). The crystal structures of closely related chalcones, *viz.*, 1-(4-bromophenyl)-3-(2,5-dimethoxyphenyl)prop-2-en-1-one, (Rosli *et al.*, 2006); 1-(4-bromophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Ng *et al.*, 2006) have been reported. Hence in continuation with the synthesis and crystal structure determination and also owing to the importance of these flavanoid analogs, this new bromo chalcone C₁₇H₁₅BrO₃ has been synthesized (Fig. 1) and its crystal structure is reported.

The title compound, C₁₇H₁₅BrO₃, is a chalcone with 2-bromophenyl and 2,5-dimethoxyphenyl rings bonded at opposite ends of a propene group (Fig. 2). The dihedral angle between mean planes of the benzene rings in the *ortho*-bromo and *ortho*-*meta*-diimethoxy substituted rings is 77.3 (1)°. The angles between the mean plane of the prop-2-ene-1-one group (C1/C7/O1/C8) and the mean planes of the benzene rings in the 2-bromophenyl (C1–C6) and 2,5-dimethoxyphenyl rings (C10–C15) are 58.6 (1)° and 30.7 (4)°, respectively. Bond distances and angles are in normal ranges (Allen *et al.*, 1987). While no classical hydrogen bonds are present, weak C3—H3···O2, C4—H4···Br1 (Tab. 1) and π -electron ring - π -electron ring interactions [$Cg1 \cdots Cg1^i = 3.650$ (2) Å; $i: -x, 1 - y, 1 - z$; Cg1 is the centroid of the ring C10–C15] are observed which contribute to the stability of crystal packing (Fig. 3).

Experimental

A 50% (wt) KOH solution (50 ml) was added to a mixture of 2-bromo acetophenone (0.01 mol, 1.99 g) and 2,5-dimethoxy benzaldehyde (0.01 mol, 1.66 g) in 25 ml of ethanol (Fig. 1). The mixture was stirred for an hour at room temperature and the precipitate was collected by filtration and purified by recrystallization from ethanol. Single crystals (triangular plates with their longest edges 0.3 - 0.5 mm long) were grown from ethyl acetate by slow evaporation method and yield of the compound was 75% (m.p. 355–357 K). Analytical data: Found (Calculated): C %: 58.76 (58.81%); H%: 4.31 (4.35%).

Refinement

All the hydrogen atoms could have been discerned in the difference electron density map, nevertheless, all the H atoms were constrained in the riding motion approximation. C_{aryl}—H = 0.95 Å, with $U_{iso}(H) = 1.20U_{eq}(C)$. C_{methyl}—H = 0.98 Å, with $U_{iso}(H) = 1.50U_{eq}(C)$.

Figures

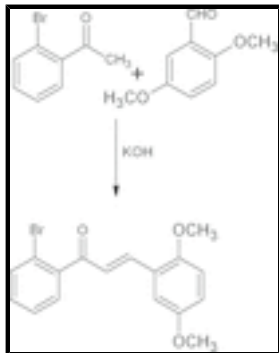


Fig. 1. Reaction scheme for $C_{17}H_{15}BrO_3$.

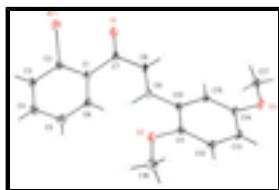


Fig. 2. Title molecule, showing the atom labelling scheme with 50% probability displacement ellipsoids.

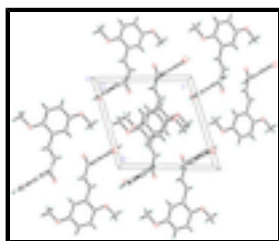


Fig. 3. Packing diagram of the title compound, $C_{17}H_{15}BrO_3$ viewed down the a axis. Dashed lines indicate a weak C—H...O intermolecular hydrogen bond interaction.

(E)-1-(2-Bromophenyl)-3-(2,5-dimethoxyphenyl)prop-2-en-1-one

Crystal data

$C_{17}H_{15}BrO_3$

$M_r = 347.20$

Triclinic, $P\bar{1}$

Hall symbol: -P 1

$a = 7.7643$ (9) Å

$b = 9.7006$ (11) Å

$c = 10.2722$ (10) Å

$\alpha = 72.901$ (10)°

$\beta = 78.487$ (9)°

$\gamma = 86.359$ (9)°

$V = 724.59$ (14) Å³

$Z = 2$

$F(000) = 352$

$D_x = 1.591$ Mg m⁻³

Melting point = 355–357 K

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 4418 reflections

$\theta = 4.6$ – 73.9 °

$\mu = 3.93$ mm⁻¹

$T = 110$ K

Triangular plate, colorless

$0.54 \times 0.26 \times 0.08$ mm

Data collection

Oxford Diffraction Xcalibur
diffractometer

Radiation source: Enhance (Cu) X-ray Source

2835 independent reflections

2749 reflections with $I > 2\sigma(I)$

graphite $R_{\text{int}} = 0.037$
 Detector resolution: 10.5081 pixels mm⁻¹ $\theta_{\text{max}} = 74.2^\circ$, $\theta_{\text{min}} = 4.6^\circ$
 ω scans $h = -9 \rightarrow 9$
 Absorption correction: analytical $k = -12 \rightarrow 11$
 (*CrysAlis RED*; Oxford Diffraction, 2007)
 $T_{\text{min}} = 0.179$, $T_{\text{max}} = 0.635$ $l = -12 \rightarrow 10$
 4759 measured reflections

Refinement

Refinement on F^2 Primary atom site location: structure-invariant direct methods
 Least-squares matrix: full Secondary atom site location: difference Fourier map
 $R[F^2 > 2\sigma(F^2)] = 0.053$ Hydrogen site location: difference Fourier map
 $wR(F^2) = 0.146$ H-atom parameters constrained
 $S = 1.05$ $w = 1/[\sigma^2(F_o^2) + (0.1005P)^2 + 1.9956P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 2835 reflections $(\Delta/\sigma)_{\text{max}} = 0.001$
 192 parameters $\Delta\rho_{\text{max}} = 2.51 \text{ e } \text{Å}^{-3}$
 0 restraints $\Delta\rho_{\text{min}} = -1.11 \text{ e } \text{Å}^{-3}$
 58 constraints

Special details

Experimental. IR data (KBr) $\nu \text{ cm}^{-1}$: 2832 cm^{-1} , 2949 cm^{-1} , 2987 cm^{-1} (C—H al. str), 3453 cm^{-1} (C—H ar. str) 1680 cm^{-1} (C=O), 1593 cm^{-1} (C=C); 1231 cm^{-1} (C—O—C).

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 $F^2 > \sigma(F^2)$ 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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.28123 (4)	1.19671 (4)	-0.00743 (4)	0.01849 (18)
O1	0.1583 (4)	1.1329 (3)	0.3257 (3)	0.0208 (6)
O2	0.4450 (3)	0.5470 (3)	0.2755 (3)	0.0161 (5)
O3	0.0011 (4)	0.4011 (3)	0.7884 (3)	0.0177 (5)
C1	0.4421 (5)	1.0666 (3)	0.2299 (4)	0.0129 (7)
C2	0.4701 (5)	1.1455 (4)	0.0894 (4)	0.0135 (7)
C3	0.6379 (5)	1.1881 (4)	0.0155 (4)	0.0160 (7)
H3	0.6548	1.2397	-0.0802	0.019*

supplementary materials

C4	0.7801 (5)	1.1552 (4)	0.0819 (4)	0.0194 (8)
H4	0.8945	1.1857	0.0318	0.023*
C5	0.7563 (5)	1.0772 (4)	0.2223 (4)	0.0203 (8)
H5	0.8536	1.0560	0.2684	0.024*
C6	0.5884 (5)	1.0312 (4)	0.2936 (4)	0.0164 (7)
H6	0.5729	0.9743	0.3878	0.020*
C7	0.2612 (5)	1.0331 (4)	0.3178 (4)	0.0138 (7)
C8	0.2125 (5)	0.8849 (4)	0.3976 (4)	0.0138 (7)
H8	0.1094	0.8697	0.4676	0.017*
C9	0.3058 (4)	0.7685 (4)	0.3774 (3)	0.0119 (6)
H9	0.4086	0.7848	0.3070	0.014*
C10	0.2606 (4)	0.6188 (3)	0.4558 (3)	0.0103 (6)
C11	0.3385 (4)	0.5059 (4)	0.4034 (3)	0.0116 (6)
C12	0.3018 (5)	0.3629 (4)	0.4806 (4)	0.0141 (7)
H12	0.3535	0.2865	0.4454	0.017*
C13	0.1900 (5)	0.3323 (4)	0.6086 (4)	0.0149 (7)
H13	0.1676	0.2348	0.6617	0.018*
C14	0.1098 (5)	0.4435 (4)	0.6606 (4)	0.0128 (7)
C15	0.1450 (4)	0.5854 (4)	0.5843 (3)	0.0116 (6)
H15	0.0903	0.6611	0.6193	0.014*
C16	0.5285 (5)	0.4359 (4)	0.2187 (4)	0.0184 (7)
H16	0.6043	0.4798	0.1291	0.028*
H16B	0.4388	0.3772	0.2057	0.028*
H16C	0.5996	0.3747	0.2825	0.028*
C17	-0.0777 (5)	0.5153 (4)	0.8422 (4)	0.0174 (7)
H17	-0.1553	0.4744	0.9317	0.026*
H17B	-0.1463	0.5775	0.7770	0.026*
H17C	0.0144	0.5721	0.8548	0.026*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0173 (3)	0.0181 (3)	0.0190 (3)	-0.00149 (16)	-0.00464 (16)	-0.00259 (16)
O1	0.0213 (13)	0.0084 (12)	0.0265 (14)	0.0010 (10)	0.0049 (11)	-0.0020 (10)
O2	0.0204 (13)	0.0086 (11)	0.0171 (12)	-0.0009 (9)	0.0051 (10)	-0.0060 (9)
O3	0.0238 (13)	0.0101 (12)	0.0131 (12)	-0.0010 (10)	0.0029 (10)	0.0021 (9)
C1	0.0176 (17)	0.0045 (14)	0.0157 (16)	-0.0038 (12)	0.0021 (13)	-0.0041 (12)
C2	0.0129 (16)	0.0104 (15)	0.0158 (16)	-0.0017 (12)	-0.0002 (13)	-0.0032 (13)
C3	0.0171 (17)	0.0103 (15)	0.0167 (16)	-0.0030 (13)	0.0031 (13)	-0.0016 (13)
C4	0.0165 (17)	0.0133 (17)	0.0248 (19)	-0.0052 (13)	0.0034 (14)	-0.0038 (14)
C5	0.0188 (18)	0.0118 (16)	0.030 (2)	-0.0014 (13)	-0.0069 (15)	-0.0042 (15)
C6	0.0220 (18)	0.0076 (15)	0.0176 (17)	-0.0005 (13)	-0.0011 (14)	-0.0021 (13)
C7	0.0173 (17)	0.0081 (15)	0.0139 (15)	-0.0034 (12)	0.0015 (13)	-0.0023 (12)
C8	0.0147 (16)	0.0076 (15)	0.0149 (16)	-0.0041 (12)	0.0044 (13)	-0.0007 (12)
C9	0.0127 (15)	0.0114 (16)	0.0106 (15)	-0.0036 (12)	0.0004 (12)	-0.0025 (12)
C10	0.0115 (15)	0.0074 (15)	0.0125 (15)	-0.0011 (11)	-0.0028 (12)	-0.0029 (12)
C11	0.0109 (15)	0.0113 (16)	0.0124 (15)	-0.0002 (12)	-0.0010 (12)	-0.0040 (12)
C12	0.0162 (16)	0.0078 (15)	0.0194 (17)	0.0016 (12)	-0.0041 (13)	-0.0053 (13)

C13	0.0180 (17)	0.0061 (15)	0.0178 (17)	-0.0027 (12)	-0.0046 (13)	0.0022 (12)
C14	0.0145 (16)	0.0090 (15)	0.0117 (15)	-0.0025 (12)	-0.0029 (12)	0.0028 (12)
C15	0.0126 (15)	0.0089 (15)	0.0127 (15)	-0.0013 (12)	-0.0016 (12)	-0.0022 (12)
C16	0.0189 (17)	0.0139 (17)	0.0225 (18)	0.0011 (13)	0.0030 (14)	-0.0107 (14)
C17	0.0183 (17)	0.0167 (17)	0.0140 (16)	-0.0010 (13)	0.0019 (13)	-0.0025 (13)

Geometric parameters (Å, °)

Br1—C2	1.893 (4)	C8—H8	0.9500
O1—C7	1.227 (4)	C9—C10	1.465 (4)
O2—C11	1.367 (4)	C9—H9	0.9500
O2—C16	1.433 (4)	C10—C15	1.402 (5)
O3—C14	1.375 (4)	C10—C11	1.410 (5)
O3—C17	1.430 (4)	C11—C12	1.396 (5)
C1—C6	1.397 (5)	C12—C13	1.384 (5)
C1—C2	1.401 (5)	C12—H12	0.9500
C1—C7	1.507 (5)	C13—C14	1.399 (5)
C2—C3	1.391 (5)	C13—H13	0.9500
C3—C4	1.383 (6)	C14—C15	1.383 (5)
C3—H3	0.9500	C15—H15	0.9500
C4—C5	1.399 (6)	C16—H16	0.9800
C4—H4	0.9500	C16—H16B	0.9800
C5—C6	1.392 (5)	C16—H16C	0.9800
C5—H5	0.9500	C17—H17	0.9800
C6—H6	0.9500	C17—H17B	0.9800
C7—C8	1.461 (4)	C17—H17C	0.9800
C8—C9	1.348 (5)		
C11—O2—C16	117.8 (3)	C15—C10—C9	121.1 (3)
C14—O3—C17	115.6 (3)	C11—C10—C9	119.5 (3)
C6—C1—C2	117.9 (3)	O2—C11—C12	124.4 (3)
C6—C1—C7	118.9 (3)	O2—C11—C10	115.8 (3)
C2—C1—C7	122.8 (3)	C12—C11—C10	119.8 (3)
C3—C2—C1	121.2 (3)	C13—C12—C11	120.0 (3)
C3—C2—Br1	117.5 (3)	C13—C12—H12	120.0
C1—C2—Br1	121.3 (3)	C11—C12—H12	120.0
C4—C3—C2	119.8 (3)	C12—C13—C14	120.7 (3)
C4—C3—H3	120.1	C12—C13—H13	119.6
C2—C3—H3	120.1	C14—C13—H13	119.6
C3—C4—C5	120.4 (3)	O3—C14—C15	124.5 (3)
C3—C4—H4	119.8	O3—C14—C13	115.9 (3)
C5—C4—H4	119.8	C15—C14—C13	119.6 (3)
C6—C5—C4	119.1 (4)	C14—C15—C10	120.6 (3)
C6—C5—H5	120.4	C14—C15—H15	119.7
C4—C5—H5	120.4	C10—C15—H15	119.7
C5—C6—C1	121.5 (3)	O2—C16—H16	109.5
C5—C6—H6	119.2	O2—C16—H16B	109.5
C1—C6—H6	119.2	H16—C16—H16B	109.5
O1—C7—C8	120.6 (3)	O2—C16—H16C	109.5
O1—C7—C1	118.9 (3)	H16—C16—H16C	109.5

supplementary materials

C8—C7—C1	120.5 (3)	H16B—C16—H16C	109.5
C9—C8—C7	123.6 (3)	O3—C17—H17	109.5
C9—C8—H8	118.2	O3—C17—H17B	109.5
C7—C8—H8	118.2	H17—C17—H17B	109.5
C8—C9—C10	124.9 (3)	O3—C17—H17C	109.5
C8—C9—H9	117.6	H17—C17—H17C	109.5
C10—C9—H9	117.6	H17B—C17—H17C	109.5
C15—C10—C11	119.3 (3)		
C6—C1—C2—C3	-0.4 (5)	C8—C9—C10—C11	163.4 (3)
C7—C1—C2—C3	172.8 (3)	C16—O2—C11—C12	-1.9 (5)
C6—C1—C2—Br1	179.1 (2)	C16—O2—C11—C10	179.4 (3)
C7—C1—C2—Br1	-7.7 (5)	C15—C10—C11—O2	177.9 (3)
C1—C2—C3—C4	-1.4 (5)	C9—C10—C11—O2	-4.0 (5)
Br1—C2—C3—C4	179.1 (3)	C15—C10—C11—C12	-0.9 (5)
C2—C3—C4—C5	1.1 (5)	C9—C10—C11—C12	177.2 (3)
C3—C4—C5—C6	1.1 (6)	O2—C11—C12—C13	-179.1 (3)
C4—C5—C6—C1	-3.0 (5)	C10—C11—C12—C13	-0.4 (5)
C2—C1—C6—C5	2.6 (5)	C11—C12—C13—C14	1.4 (5)
C7—C1—C6—C5	-170.8 (3)	C17—O3—C14—C15	-0.1 (5)
C6—C1—C7—O1	117.6 (4)	C17—O3—C14—C13	178.8 (3)
C2—C1—C7—O1	-55.5 (5)	C12—C13—C14—O3	179.9 (3)
C6—C1—C7—C8	-59.4 (4)	C12—C13—C14—C15	-1.1 (5)
C2—C1—C7—C8	127.4 (4)	O3—C14—C15—C10	178.7 (3)
O1—C7—C8—C9	168.8 (4)	C13—C14—C15—C10	-0.2 (5)
C1—C7—C8—C9	-14.3 (5)	C11—C10—C15—C14	1.2 (5)
C7—C8—C9—C10	179.9 (3)	C9—C10—C15—C14	-176.8 (3)
C8—C9—C10—C15	-18.5 (5)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C4—H4 \cdots Br1 ⁱ	0.95	2.95	3.834 (4)	155
C3—H3 \cdots O2 ⁱⁱ	0.95	2.62	3.463 (5)	148

Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, -y+2, -z$.

Fig. 1

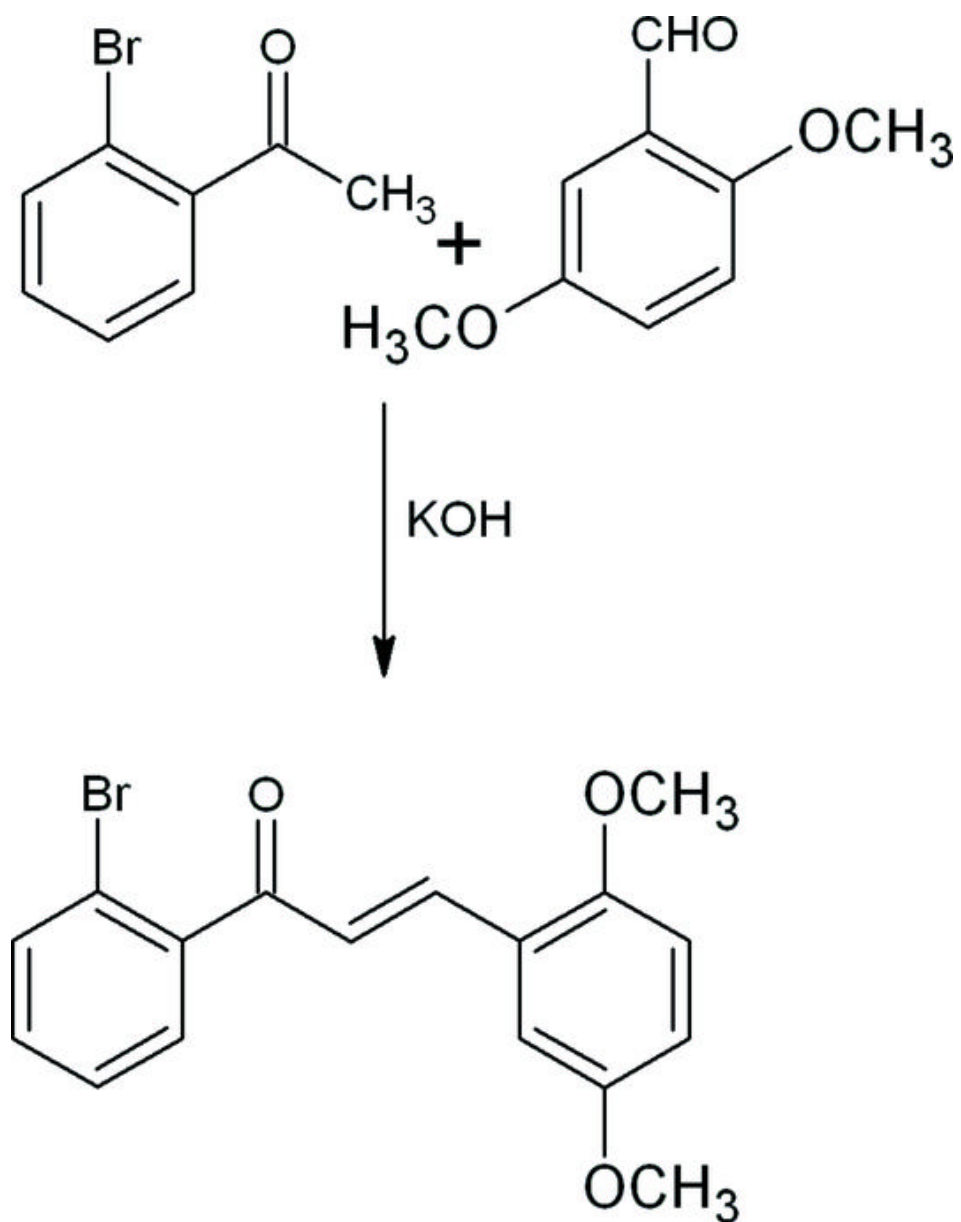


Fig. 2

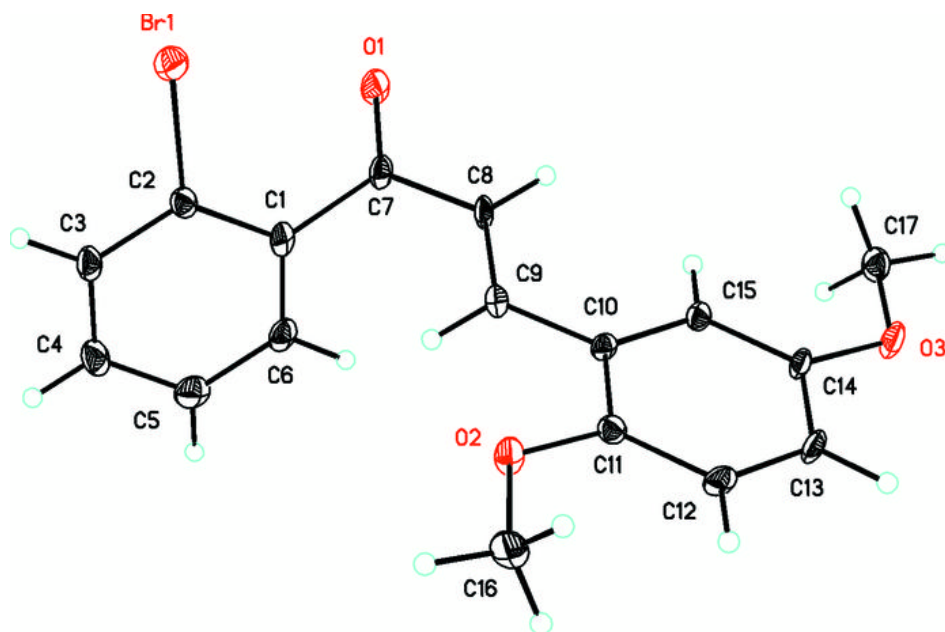


Fig. 3

