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1-(4-Bromophenyl)-3-(3-methoxyphenyl)prop-2-en-1-one

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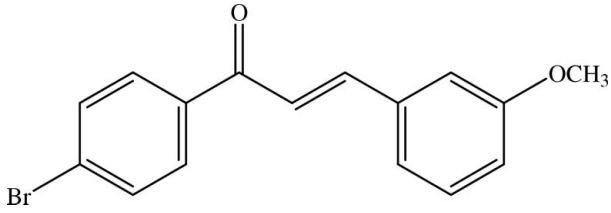
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.075; data-to-parameter ratio = 27.7.

The title compound, $C_{16}H_{13}BrO_2$, crystallizes with two independent molecules (A and B) in the asymmetric unit. The dihedral angle between the two benzene rings is 45.94 (8)° in molecule A and 46.82 (7)° in molecule B. The crystal packing is stabilized by weak C—H···π interactions.

Related literature

For bond length data, see: Allen *et al.* (1987). For related literature, see: Patil, Chantrapromma *et al.* (2007); Patil, Dharmaprakash *et al.* (2006); Patil, Ng *et al.* (2007); Patil, Rosli *et al.* (2007); Patil, Teh *et al.* (2006); Shettigar *et al.* (2006).



Experimental

Crystal data

$C_{16}H_{13}BrO_2$
M_r = 317.17
Triclinic, $P\overline{1}$
a = 5.8459 (1) Å
b = 7.3649 (2) Å
c = 31.1430 (8) Å
α = 83.866 (1)°
β = 87.023 (1)°
γ = 85.297 (1)°
V = 1327.42 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.09 mm^{-1}
T = 100.0 (1) K
0.57 × 0.40 × 0.32 mm

Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.273, T_{max} = 0.439
(expected range = 0.231–0.372)
35306 measured reflections
9572 independent reflections
7816 reflections with $I > 2\sigma(I)$
R_{int} = 0.030

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.075
S = 1.04
9572 reflections
345 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.55 e Å^{-3}
$\Delta\rho_{min}$ = −0.81 e Å^{-3}

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

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 denote the centroids of the rings C1*A*–C6*A*, C10*A*–C15*A*, C1*B*–C6*B* and C10*B*–C15*B*, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C2*A*—H2*AA*···*Cg*2^{i}	0.93	2.86	3.4495 (17)	123
C5*A*—H5*AA*···*Cg*2^{ii}	0.93	2.77	3.3798 (17)	124
C2*B*—H2*BA*···*Cg*4^{iii}	0.93	2.97	3.5305 (16)	120
C5*B*—H5*BA*···*Cg*4^{iv}	0.93	2.88	3.4596 (17)	122
C14*A*—H14*A*···*Cg*1^{v}	0.93	2.86	3.5094 (17)	128
C14*B*—H14*B*···*Cg*3^{vi}	0.93	2.69	3.3678 (17)	131

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

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2364).

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supplementary materials

Acta Cryst. (2007). E**63**, o2612 [**doi:10.1107/S1600536807018648**]

1-(4-Bromophenyl)-3-(3-methoxyphenyl)prop-2-en-1-one

P. S. Patil, S. Chantrapromma, H.-K. Fun, S. M. Dharmaprakash and H. B. R. Babu

Comment

Chalcone derivatives have been synthesized by us to study their nonlinear optical properties, since they are prominent materials with excellent blue-light transmittance and good crystallizability (Patil, Teh *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2006; Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2007; Patil, Rosli *et al.*, 2007; Patil, Chantrapromma *et al.*, 2007). The single-crystal X-ray structural study of the title compound, (I), was undertaken in order to establish the structure and conformation of the various groups. Crystallization of compound (I) in a centrosymmetric space group precludes second-order nonlinear optical properties.

There are two independent molecules, *A* and *B*, in the asymmetric unit of (I) (Fig. 1). Bond lengths and angles in (I) are in normal ranges (Allen *et al.*, 1987) and comparable with those in related structures (Patil, Teh *et al.*, 2006; Patil, Dharmaprakash *et al.*, 2006; Shettigar *et al.*, 2006; Patil, Ng *et al.*, 2007; Patil, Chantrapromma *et al.*, 2007). The dihedral angle between the two benzene rings is 45.94 (8)° in molecule *A* and 46.82 (7)°

in molecule *B*. In molecule *A*, the least-squares plane through the

O1/C6/C7/C8 group makes dihedral angles of 28.83 (9) and 21.34 (9)° with the C1–C6 and C10–C15 benzene rings, repectively; the corresponding values are 27.56 (9) and 23.85 (9)°, respectively, in molecule *B*.

A view of the molecular packing in the crystal structure is shown in Fig. 2. The crystal packing is stabilized by weak C—H···π interactions (Table 1; Cg1, Cg2, Cg3 and Cg4 denote the centroids of the rings C1A–C6A, C10A–C15A, C1B–C6B and C10B–C15B, respectively).

Experimental

3-Methoxybenzaldehyde (0.01 mol) and 4-bromoacetophenone (0.01 mol) were stirred in methanol (60 ml) at room temperature. 10% NaOH aqueous solution (5 g) was added and the mixture was stirred for 4 h. The resulting precipitate was filtered off, washed with water and dried. The resulting crude product was recrystallized from acetone. Colourless block-shaped single crystals of (I) suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Refinement

All H atoms were positioned geometrically and allowed to ride on their parent atoms, with C—H distances in the range 0.93–0.96 Å and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(C)

for the remaining H atoms. A rotating-group model was used for the methyl group.

Figures

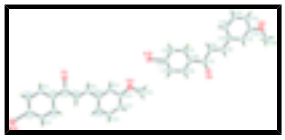


Fig. 1. The asymmetric unit of (I), showing the atomic numbering scheme and with 80% probability displacement ellipsoids.

Fig. 2. The crystal packing of (I), viewed down the *a* axis.

1-(4-bromophenyl)-3-(3-methoxyphenyl)prop-2-en-1-one

Crystal data

$C_{16}H_{13}BrO_2$	$Z = 4$
$M_r = 317.17$	$F_{000} = 640$
Triclinic, $P\overline{1}$	$D_x = 1.587$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.8459$ (1) Å	Cell parameters from 9572 reflections
$b = 7.3649$ (2) Å	$\theta = 0.7$–32.5°
$c = 31.1430$ (8) Å	$\mu = 3.09$ mm^{-1}
$\alpha = 83.866$ (1)°	$T = 100.0$ (1) K
$\beta = 87.023$ (1)°	Block, colourless
$\gamma = 85.297$ (1)°	0.57 × 0.40 × 0.32 mm
$V = 1327.42$ (5) Å^3	

Data collection

Bruker SMART APEXII CCD area-detector diffractometer	9572 independent reflections
Radiation source: fine-focus sealed tube	7816 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.030$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 32.5^\circ$
$T = 100.0(1)$ K	$\theta_{min} = 0.7^\circ$
ω scans	$h = -8 \rightarrow 8$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -11 \rightarrow 11$
$T_{min} = 0.273$, $T_{max} = 0.439$	$l = -47 \rightarrow 47$
35306 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0228P)^2 + 1.5366P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.034$	$(\Delta/\sigma)_{max} = 0.002$

$wR(F^2) = 0.075$

$S = 1.04$

9572 reflections

345 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

$\Delta\rho_{max} = 0.55$ e Å^{-3}

$\Delta\rho_{min} = -0.81$ 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 $F^2 > 2\text{sigma}(F^2)$ 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	0.84725 (3)	0.07145 (3)	−0.205507 (6)	0.02172 (5)
O1A	0.2884 (2)	0.21055 (19)	−0.01168 (4)	0.0204 (3)
O2A	0.6853 (3)	0.3419 (2)	0.20030 (4)	0.0254 (3)
C1A	0.8077 (3)	0.0967 (2)	−0.07324 (6)	0.0165 (3)
H1AA	0.9060	0.0692	−0.0505	0.020*
C2A	0.8833 (3)	0.0624 (2)	−0.11480 (6)	0.0170 (3)
H2AA	1.0306	0.0092	−0.1200	0.020*
C3A	0.7361 (3)	0.1088 (2)	−0.14859 (5)	0.0163 (3)
C4A	0.5133 (3)	0.1835 (2)	−0.14150 (6)	0.0178 (3)
H4AA	0.4166	0.2133	−0.1644	0.021*
C5A	0.4373 (3)	0.2129 (2)	−0.09972 (6)	0.0166 (3)
H5AA	0.2872	0.2600	−0.0945	0.020*
C6A	0.5841 (3)	0.1723 (2)	−0.06541 (5)	0.0147 (3)
C7A	0.4952 (3)	0.2110 (2)	−0.02116 (5)	0.0154 (3)
C8A	0.6620 (3)	0.2555 (2)	0.00939 (6)	0.0175 (3)
H8AA	0.8125	0.2735	−0.0003	0.021*
C9A	0.5984 (3)	0.2703 (2)	0.05092 (6)	0.0158 (3)
H9AA	0.4490	0.2440	0.0595	0.019*
C10A	0.7409 (3)	0.3237 (2)	0.08403 (5)	0.0148 (3)
C11A	0.6590 (3)	0.3073 (2)	0.12715 (6)	0.0161 (3)
H11A	0.5181	0.2593	0.1343	0.019*
C12A	0.7854 (3)	0.3620 (2)	0.15958 (6)	0.0181 (3)
C13A	0.9971 (3)	0.4331 (3)	0.14927 (6)	0.0192 (3)

H13A	1.0830	0.4694	0.1707	0.023*
C14A	1.0781 (3)	0.4489 (2)	0.10627 (6)	0.0185 (3)
H14A	1.2192	0.4968	0.0993	0.022*
C15A	0.9548 (3)	0.3956 (2)	0.07379 (6)	0.0167 (3)
H15A	1.0128	0.4071	0.0453	0.020*
C16A	0.8057 (4)	0.4059 (3)	0.23368 (7)	0.0296 (4)
H16A	0.7184	0.3889	0.2606	0.044*
H16B	0.8272	0.5337	0.2267	0.044*
H16C	0.9527	0.3382	0.2363	0.044*
Br1B	0.23024 (3)	0.57967 (3)	0.299714 (6)	0.02259 (5)
O1B	0.7133 (2)	0.28906 (19)	0.49324 (4)	0.0207 (3)
O2B	0.1579 (2)	−0.0121 (2)	0.70895 (4)	0.0231 (3)
C1B	0.2181 (3)	0.4494 (2)	0.43231 (6)	0.0168 (3)
H1BA	0.1101	0.4569	0.4552	0.020*
C2B	0.1585 (3)	0.5166 (2)	0.39075 (6)	0.0167 (3)
H2BA	0.0125	0.5722	0.3857	0.020*
C3B	0.3193 (3)	0.4997 (2)	0.35684 (6)	0.0161 (3)
C4B	0.5420 (3)	0.4240 (2)	0.36360 (6)	0.0170 (3)
H4BA	0.6489	0.4155	0.3406	0.020*
C5B	0.6012 (3)	0.3613 (2)	0.40554 (6)	0.0160 (3)
H5BA	0.7502	0.3126	0.4107	0.019*
C6B	0.4393 (3)	0.3708 (2)	0.43998 (5)	0.0144 (3)
C7B	0.5106 (3)	0.2960 (2)	0.48421 (6)	0.0162 (3)
C8B	0.3309 (3)	0.2270 (2)	0.51541 (6)	0.0176 (3)
H8BA	0.1864	0.2125	0.5057	0.021*
C9B	0.3712 (3)	0.1849 (2)	0.55731 (5)	0.0157 (3)
H9BA	0.5138	0.2091	0.5663	0.019*
C10B	0.2108 (3)	0.1040 (2)	0.59027 (5)	0.0150 (3)
C11B	0.2677 (3)	0.0902 (2)	0.63390 (5)	0.0156 (3)
H11B	0.4023	0.1355	0.6414	0.019*
C12B	0.1220 (3)	0.0086 (2)	0.66576 (6)	0.0167 (3)
C13B	−0.0778 (3)	−0.0626 (2)	0.65429 (6)	0.0185 (3)
H13B	−0.1724	−0.1211	0.6754	0.022*
C14B	−0.1347 (3)	−0.0459 (2)	0.61143 (6)	0.0174 (3)
H14B	−0.2696	−0.0911	0.6040	0.021*
C15B	0.0068 (3)	0.0375 (2)	0.57933 (6)	0.0164 (3)
H15B	−0.0341	0.0491	0.5506	0.020*
C16B	0.3534 (4)	0.0636 (4)	0.72329 (7)	0.0320 (5)
H16D	0.4902	0.0109	0.7096	0.048*
H16E	0.3604	0.0372	0.7541	0.048*
H16F	0.3415	0.1939	0.7159	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1A	0.02332 (9)	0.02702 (10)	0.01429 (8)	0.00146 (7)	0.00084 (6)	−0.00305 (6)
O1A	0.0156 (6)	0.0263 (7)	0.0194 (6)	−0.0016 (5)	0.0007 (5)	−0.0042 (5)
O2A	0.0286 (7)	0.0341 (8)	0.0140 (6)	−0.0040 (6)	0.0008 (5)	−0.0050 (5)

C1A	0.0157 (7)	0.0178 (8)	0.0155 (7)	0.0001 (6)	−0.0015 (6)	−0.0004 (6)
C2A	0.0155 (7)	0.0174 (8)	0.0177 (8)	0.0007 (6)	−0.0012 (6)	−0.0012 (6)
C3A	0.0186 (8)	0.0163 (8)	0.0139 (7)	−0.0014 (6)	0.0005 (6)	−0.0022 (6)
C4A	0.0175 (8)	0.0187 (8)	0.0175 (8)	0.0008 (6)	−0.0041 (6)	−0.0025 (6)
C5A	0.0139 (7)	0.0171 (8)	0.0191 (8)	−0.0009 (6)	−0.0014 (6)	−0.0025 (6)
C6A	0.0159 (7)	0.0122 (7)	0.0160 (7)	−0.0028 (6)	0.0006 (6)	−0.0013 (6)
C7A	0.0167 (7)	0.0142 (7)	0.0154 (7)	−0.0012 (6)	−0.0005 (6)	−0.0015 (6)
C8A	0.0163 (7)	0.0187 (8)	0.0177 (8)	−0.0025 (6)	−0.0006 (6)	−0.0024 (6)
C9A	0.0151 (7)	0.0143 (7)	0.0181 (7)	−0.0010 (6)	−0.0012 (6)	−0.0021 (6)
C10A	0.0159 (7)	0.0134 (7)	0.0151 (7)	0.0004 (6)	−0.0009 (6)	−0.0020 (6)
C11A	0.0159 (7)	0.0147 (7)	0.0174 (7)	−0.0007 (6)	0.0004 (6)	−0.0015 (6)
C12A	0.0207 (8)	0.0171 (8)	0.0160 (7)	0.0014 (6)	−0.0013 (6)	−0.0020 (6)
C13A	0.0208 (8)	0.0183 (8)	0.0188 (8)	−0.0005 (6)	−0.0056 (6)	−0.0025 (6)
C14A	0.0156 (7)	0.0169 (8)	0.0230 (8)	−0.0016 (6)	−0.0014 (6)	−0.0012 (6)
C15A	0.0167 (7)	0.0160 (8)	0.0170 (7)	−0.0009 (6)	−0.0002 (6)	−0.0009 (6)
C16A	0.0408 (12)	0.0316 (11)	0.0176 (9)	−0.0019 (9)	−0.0043 (8)	−0.0074 (8)
Br1B	0.02450 (9)	0.02607 (10)	0.01655 (8)	−0.00148 (7)	−0.00473 (6)	0.00236 (7)
O1B	0.0165 (6)	0.0268 (7)	0.0189 (6)	−0.0023 (5)	−0.0033 (5)	−0.0008 (5)
O2B	0.0220 (6)	0.0318 (8)	0.0157 (6)	−0.0066 (5)	−0.0009 (5)	0.0001 (5)
C1B	0.0162 (7)	0.0173 (8)	0.0173 (7)	−0.0011 (6)	0.0005 (6)	−0.0045 (6)
C2B	0.0143 (7)	0.0153 (8)	0.0207 (8)	0.0002 (6)	−0.0025 (6)	−0.0028 (6)
C3B	0.0187 (8)	0.0140 (7)	0.0157 (7)	−0.0025 (6)	−0.0021 (6)	−0.0004 (6)
C4B	0.0170 (7)	0.0173 (8)	0.0164 (7)	−0.0013 (6)	0.0014 (6)	−0.0015 (6)
C5B	0.0144 (7)	0.0157 (8)	0.0177 (7)	−0.0012 (6)	−0.0010 (6)	−0.0012 (6)
C6B	0.0152 (7)	0.0134 (7)	0.0153 (7)	−0.0026 (6)	−0.0011 (5)	−0.0029 (5)
C7B	0.0185 (8)	0.0149 (7)	0.0157 (7)	−0.0020 (6)	−0.0008 (6)	−0.0029 (6)
C8B	0.0170 (7)	0.0188 (8)	0.0173 (8)	−0.0041 (6)	−0.0009 (6)	−0.0009 (6)
C9B	0.0161 (7)	0.0144 (7)	0.0167 (7)	−0.0008 (6)	−0.0004 (6)	−0.0025 (6)
C10B	0.0152 (7)	0.0136 (7)	0.0161 (7)	0.0004 (6)	−0.0009 (6)	−0.0023 (6)
C11B	0.0150 (7)	0.0159 (8)	0.0162 (7)	−0.0013 (6)	−0.0004 (6)	−0.0024 (6)
C12B	0.0169 (7)	0.0164 (8)	0.0164 (7)	−0.0002 (6)	−0.0002 (6)	−0.0014 (6)
C13B	0.0173 (8)	0.0165 (8)	0.0213 (8)	−0.0027 (6)	0.0029 (6)	−0.0014 (6)
C14B	0.0152 (7)	0.0147 (8)	0.0227 (8)	−0.0015 (6)	−0.0013 (6)	−0.0035 (6)
C15B	0.0160 (7)	0.0149 (8)	0.0187 (8)	0.0001 (6)	−0.0021 (6)	−0.0030 (6)
C16B	0.0212 (9)	0.0568 (15)	0.0201 (9)	−0.0081 (9)	−0.0009 (7)	−0.0101 (9)

Geometric parameters (Å, °)

Br1A—C3A	1.8960 (17)	Br1B—C3B	1.8987 (17)
O1A—C7A	1.230 (2)	O1B—C7B	1.228 (2)
O2A—C12A	1.367 (2)	O2B—C12B	1.363 (2)
O2A—C16A	1.426 (2)	O2B—C16B	1.424 (3)
C1A—C2A	1.388 (2)	C1B—C2B	1.387 (2)
C1A—C6A	1.398 (2)	C1B—C6B	1.394 (2)
C1A—H1AA	0.93	C1B—H1BA	0.93
C2A—C3A	1.390 (2)	C2B—C3B	1.385 (2)
C2A—H2AA	0.93	C2B—H2BA	0.93
C3A—C4A	1.388 (2)	C3B—C4B	1.391 (2)
C4A—C5A	1.386 (2)	C4B—C5B	1.389 (2)

C4A—H4AA	0.93	C4B—H4BA	0.93
C5A—C6A	1.397 (2)	C5B—C6B	1.397 (2)
C5A—H5AA	0.93	C5B—H5BA	0.93
C6A—C7A	1.495 (2)	C6B—C7B	1.494 (2)
C7A—C8A	1.476 (2)	C7B—C8B	1.477 (2)
C8A—C9A	1.340 (2)	C8B—C9B	1.337 (2)
C8A—H8AA	0.93	C8B—H8BA	0.93
C9A—C10A	1.464 (2)	C9B—C10B	1.466 (2)
C9A—H9AA	0.93	C9B—H9BA	0.93
C10A—C11A	1.398 (2)	C10B—C15B	1.397 (2)
C10A—C15A	1.406 (2)	C10B—C11B	1.407 (2)
C11A—C12A	1.394 (2)	C11B—C12B	1.393 (2)
C11A—H11A	0.93	C11B—H11B	0.93
C12A—C13A	1.392 (3)	C12B—C13B	1.397 (3)
C13A—C14A	1.393 (3)	C13B—C14B	1.383 (3)
C13A—H13A	0.93	C13B—H13B	0.93
C14A—C15A	1.380 (3)	C14B—C15B	1.388 (2)
C14A—H14A	0.93	C14B—H14B	0.93
C15A—H15A	0.93	C15B—H15B	0.93
C16A—H16A	0.96	C16B—H16D	0.96
C16A—H16B	0.96	C16B—H16E	0.96
C16A—H16C	0.96	C16B—H16F	0.96
C12A—O2A—C16A	116.41 (16)	C12B—O2B—C16B	117.92 (15)
C2A—C1A—C6A	120.24 (16)	C2B—C1B—C6B	120.29 (16)
C2A—C1A—H1AA	119.9	C2B—C1B—H1BA	119.9
C6A—C1A—H1AA	119.9	C6B—C1B—H1BA	119.9
C1A—C2A—C3A	119.15 (16)	C3B—C2B—C1B	119.19 (16)
C1A—C2A—H2AA	120.4	C3B—C2B—H2BA	120.4
C3A—C2A—H2AA	120.4	C1B—C2B—H2BA	120.4
C4A—C3A—C2A	121.51 (16)	C2B—C3B—C4B	121.72 (16)
C4A—C3A—Br1A	119.93 (13)	C2B—C3B—Br1B	118.76 (13)
C2A—C3A—Br1A	118.55 (13)	C4B—C3B—Br1B	119.52 (13)
C5A—C4A—C3A	118.90 (16)	C5B—C4B—C3B	118.48 (16)
C5A—C4A—H4AA	120.5	C5B—C4B—H4BA	120.8
C3A—C4A—H4AA	120.5	C3B—C4B—H4BA	120.8
C4A—C5A—C6A	120.66 (16)	C4B—C5B—C6B	120.73 (16)
C4A—C5A—H5AA	119.7	C4B—C5B—H5BA	119.6
C6A—C5A—H5AA	119.7	C6B—C5B—H5BA	119.6
C5A—C6A—C1A	119.50 (16)	C1B—C6B—C5B	119.52 (16)
C5A—C6A—C7A	118.48 (15)	C1B—C6B—C7B	122.08 (15)
C1A—C6A—C7A	122.03 (15)	C5B—C6B—C7B	118.40 (15)
O1A—C7A—C8A	122.18 (16)	O1B—C7B—C8B	122.20 (16)
O1A—C7A—C6A	120.01 (15)	O1B—C7B—C6B	120.13 (16)
C8A—C7A—C6A	117.78 (15)	C8B—C7B—C6B	117.64 (15)
C9A—C8A—C7A	120.57 (16)	C9B—C8B—C7B	121.50 (16)
C9A—C8A—H8AA	119.7	C9B—C8B—H8BA	119.3
C7A—C8A—H8AA	119.7	C7B—C8B—H8BA	119.3
C8A—C9A—C10A	126.44 (16)	C8B—C9B—C10B	125.81 (16)
C8A—C9A—H9AA	116.8	C8B—C9B—H9BA	117.1

C10A—C9A—H9AA	116.8	C10B—C9B—H9BA	117.1
C11A—C10A—C15A	118.87 (16)	C15B—C10B—C11B	119.60 (16)
C11A—C10A—C9A	118.94 (15)	C15B—C10B—C9B	121.75 (15)
C15A—C10A—C9A	122.17 (15)	C11B—C10B—C9B	118.64 (15)
C12A—C11A—C10A	120.94 (16)	C12B—C11B—C10B	119.85 (16)
C12A—C11A—H11A	119.5	C12B—C11B—H11B	120.1
C10A—C11A—H11A	119.5	C10B—C11B—H11B	120.1
O2A—C12A—C13A	124.65 (17)	O2B—C12B—C11B	125.29 (16)
O2A—C12A—C11A	115.38 (16)	O2B—C12B—C13B	114.70 (15)
C13A—C12A—C11A	119.96 (16)	C11B—C12B—C13B	120.01 (16)
C12A—C13A—C14A	118.87 (17)	C14B—C13B—C12B	119.83 (16)
C12A—C13A—H13A	120.6	C14B—C13B—H13B	120.1
C14A—C13A—H13A	120.6	C12B—C13B—H13B	120.1
C15A—C14A—C13A	121.84 (17)	C13B—C14B—C15B	120.89 (16)
C15A—C14A—H14A	119.1	C13B—C14B—H14B	119.6
C13A—C14A—H14A	119.1	C15B—C14B—H14B	119.6
C14A—C15A—C10A	119.52 (16)	C14B—C15B—C10B	119.78 (16)
C14A—C15A—H15A	120.2	C14B—C15B—H15B	120.1
C10A—C15A—H15A	120.2	C10B—C15B—H15B	120.1
O2A—C16A—H16A	109.5	O2B—C16B—H16D	109.5
O2A—C16A—H16B	109.5	O2B—C16B—H16E	109.5
H16A—C16A—H16B	109.5	H16D—C16B—H16E	109.5
O2A—C16A—H16C	109.5	O2B—C16B—H16F	109.5
H16A—C16A—H16C	109.5	H16D—C16B—H16F	109.5
H16B—C16A—H16C	109.5	H16E—C16B—H16F	109.5
C6A—C1A—C2A—C3A	1.7 (3)	C6B—C1B—C2B—C3B	1.9 (3)
C1A—C2A—C3A—C4A	−1.9 (3)	C1B—C2B—C3B—C4B	−2.7 (3)
C1A—C2A—C3A—Br1A	177.12 (13)	C1B—C2B—C3B—Br1B	176.50 (13)
C2A—C3A—C4A—C5A	0.3 (3)	C2B—C3B—C4B—C5B	1.1 (3)
Br1A—C3A—C4A—C5A	−178.73 (13)	Br1B—C3B—C4B—C5B	−178.07 (13)
C3A—C4A—C5A—C6A	1.6 (3)	C3B—C4B—C5B—C6B	1.3 (3)
C4A—C5A—C6A—C1A	−1.8 (3)	C2B—C1B—C6B—C5B	0.5 (3)
C4A—C5A—C6A—C7A	178.50 (16)	C2B—C1B—C6B—C7B	−179.74 (16)
C2A—C1A—C6A—C5A	0.1 (3)	C4B—C5B—C6B—C1B	−2.1 (3)
C2A—C1A—C6A—C7A	179.84 (16)	C4B—C5B—C6B—C7B	178.13 (16)
C5A—C6A—C7A—O1A	27.0 (2)	C1B—C6B—C7B—O1B	−153.84 (18)
C1A—C6A—C7A—O1A	−152.69 (17)	C5B—C6B—C7B—O1B	25.9 (2)
C5A—C6A—C7A—C8A	−150.78 (16)	C1B—C6B—C7B—C8B	28.0 (2)
C1A—C6A—C7A—C8A	29.5 (2)	C5B—C6B—C7B—C8B	−152.18 (16)
O1A—C7A—C8A—C9A	10.1 (3)	O1B—C7B—C8B—C9B	12.6 (3)
C6A—C7A—C8A—C9A	−172.12 (16)	C6B—C7B—C8B—C9B	−169.30 (16)
C7A—C8A—C9A—C10A	−176.23 (16)	C7B—C8B—C9B—C10B	−175.57 (16)
C8A—C9A—C10A—C11A	−171.02 (17)	C8B—C9B—C10B—C15B	9.6 (3)
C8A—C9A—C10A—C15A	10.7 (3)	C8B—C9B—C10B—C11B	−171.76 (17)
C15A—C10A—C11A—C12A	0.4 (3)	C15B—C10B—C11B—C12B	0.8 (3)
C9A—C10A—C11A—C12A	−177.94 (16)	C9B—C10B—C11B—C12B	−177.94 (16)
C16A—O2A—C12A—C13A	2.5 (3)	C16B—O2B—C12B—C11B	3.4 (3)
C16A—O2A—C12A—C11A	−176.78 (17)	C16B—O2B—C12B—C13B	−177.54 (18)
C10A—C11A—C12A—O2A	178.96 (16)	C10B—C11B—C12B—O2B	−179.75 (17)

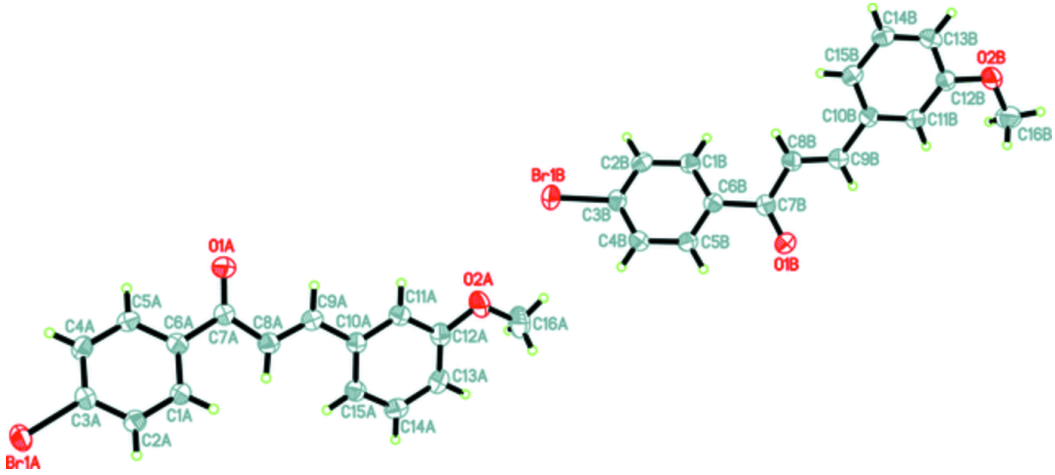
C10A—C11A—C12A—C13A	−0.4 (3)	C10B—C11B—C12B—C13B	1.3 (3)
O2A—C12A—C13A—C14A	−178.98 (17)	O2B—C12B—C13B—C14B	178.57 (16)
C11A—C12A—C13A—C14A	0.3 (3)	C11B—C12B—C13B—C14B	−2.4 (3)
C12A—C13A—C14A—C15A	−0.2 (3)	C12B—C13B—C14B—C15B	1.4 (3)
C13A—C14A—C15A—C10A	0.2 (3)	C13B—C14B—C15B—C10B	0.7 (3)
C11A—C10A—C15A—C14A	−0.3 (3)	C11B—C10B—C15B—C14B	−1.7 (3)
C9A—C10A—C15A—C14A	177.95 (16)	C9B—C10B—C15B—C14B	176.94 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2A—H2AA···Cg2^{i}	0.93	2.86	3.4495 (17)	123
C5A—H5AA···Cg2^{ii}	0.93	2.77	3.3798 (17)	124
C2B—H2BA···Cg4^{iii}	0.93	2.97	3.5305 (16)	120
C5B—H5BA···Cg4^{iv}	0.93	2.88	3.4596 (17)	122
C14A—H14A···Cg1^{v}	0.93	2.86	3.5094 (17)	128
C14B—H14B···Cg3^{vi}	0.93	2.69	3.3678 (17)	131

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

Fig. 1


C14B
C13B
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C6B
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C11A
C4A
C6A
C7A
C8A
C10A
C12A
C16A
C13A
C3A
C1A
C15A
C2A
C14A
Br1A

Fig. 2