Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Bromo-1-chlorophenyl-3-(4-methoxyphenyl)prop-2-en-1-one

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.002 Å
R factor = 0.024
wR factor = 0.060
Data-to-parameter ratio = 17.8

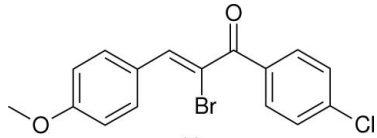
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 21 March 2006
Accepted 22 March 2006

The geometrical parameters for the title compound, $C_{16}H_{12}BrClO_2$, are normal. The observed bond lengths and angles imply that there is little electronic conjugation between the two benzene ring systems. An intramolecular C—H···Br interaction may help to establish the molecular conformation. The crystal packing results in a centrosymmetric structure.

Comment

Many chalcone ($C_{15}H_{12}O$) derivatives crystallize as non-centrosymmetric structures and display significant non-linear optical (NLO) properties (Uchida *et al.*, 1998). The title compound, (I), (Fig. 1), was prepared as part of our ongoing studies in this area (Harrison *et al.*, 2005). However, (I) crystallizes in a centrosymmetric space group, thus it has a zero NLO response (Watson *et al.*, 1993).



(I)

The geometrical parameters for (I) are normal (Allen *et al.*, 1987) and consistent with those of other chalcone derivatives (Moorthi *et al.*, 2005; Patil *et al.*, 2006). The molecule of (I) is distinctly twisted about the C4—C7 and C7—C8 bonds (Table 1). This twisting, and the C4—C7 and C7—C8 bond lengths of greater than 1.48 Å, imply that there is limited electronic conjugation between the two aromatic ring systems. The dihedral angle between the benzene ring mean planes (C1–C6 and C10–C15) is 53.35 (6)°. C7 and O2 deviate from the former mean plane by 0.176 (3) and 0.895 (3) Å, respectively. By contrast, the terminal methyl atom C16 is almost coplanar with the C10–C15 ring [deviation = 0.045 (4) Å].

A *PLATON* (Spek, 2003) analysis of (I) indicated a possible intramolecular C—H···Br interaction (Table 2) that might help to maintain near coplanarity between the C8/C9/Br1 fragment and the C10-benzene ring. The predicted (Bondi, 1964) van der Waals contact distance for H and Br is 3.05 Å. There are no π···π stacking interactions in the crystal structure of (I).

Experimental

2,3-Dibromo-1-chlorophenyl-3-(4-methoxyphenyl)-2-propan-1-one (4.32 g, 0.01 mol) was mixed with triethylamine (5 ml, 0.05 mol) in toluene (100 ml). The reaction was stirred for 24 hrs. and the precipitated triethylamine hydrobromide was removed by filtration.

The solvent was removed under reduced pressure and the resulting solid mass obtained on cooling was collected by filtration. The crude product was recrystallized from ethanol to yield blocks of (I) in 60% yield. M.p.: 403 K. Analysis for $C_{16}H_{12}BrClO_2$: calc. C 54.65, H 3.44%, found: C 54.53, H 3.64%.

Crystal data

$C_{16}H_{12}BrClO_2$
M_r = 351.62
Monoclinic, $P2_1/c$
a = 13.9793 (3) Å
b = 8.8780 (1) Å
c = 11.4870 (3) Å
β = 96.7094 (10)°
V = 1415.87 (5) Å^3
Z = 4
D_x = 1.650 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3426 reflections
θ = 2.9–27.5°
μ = 3.09 mm^{-1}
T = 120 (2) K
Block, colourless
0.55 × 0.37 × 0.18 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: multi-scan *SADABS* (Bruker, 2003)
T_{min} = 0.266, T_{max} = 0.573
19150 measured reflections
3249 independent reflections
2906 reflections with $I > 2\sigma(I)$
R_{int} = 0.039
θ_{max} = 27.5°
$h = -18 \rightarrow 18$
$k = -11 \rightarrow 11$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.024
$wR(F^2)$ = 0.060
S = 1.04
3249 reflections
183 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0257P)^2 + 1.1891P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.58 e Å^{-3}
Extinction correction: *SHELXL*
Extinction coefficient: 0.0135 (6)

Table 1
Selected geometric parameters (Å, °).

C4—C7	1.494 (2)	C8—C9	1.346 (2)
C7—C8	1.488 (2)	C9—C10	1.460 (2)
C3—C4—C7—O2	33.7 (2)	C8—C9—C10—C15	−2.9 (3)
O2—C7—C8—Br1	19.6 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···Br1	0.95	2.62	3.3339 (18)	132

H atoms were positioned geometrically (C—H = 0.95–0.98 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(carrier) or 1.5U_{eq}(methyl carrier). The methyl group was rotated to fit the electron density.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *HKL SCALEPACK* (Otwinowski & Minor 1997); data reduction: *HKL SCALEPACK* and *DENZO* (Otwinowski & Minor 1997), *SCALEPACK* and *SORTAV* (Blessing 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

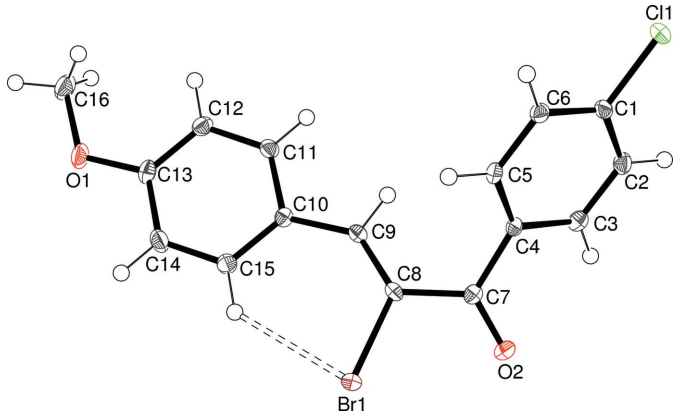


Figure 1
View of (I), showing 50% displacement ellipsoids (arbitrary spheres for the H atoms). The possible C—H···Br interaction is indicated by a dashed line.

We thank the EPSRC National Crystallography Service (University of Southampton) for the data collection. One of the authors (BKS) thanks AICTE, Government of India, New Delhi for financial assistance under the 'Career Award for Young Teachers' Scheme.

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