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3-(Biphenyl-4-yl)-2,3-dibromo-1-(2,4-dichlorophenyl)propan-1-one

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Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.037
wR factor = 0.091
Data-to-parameter ratio = 24.8

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

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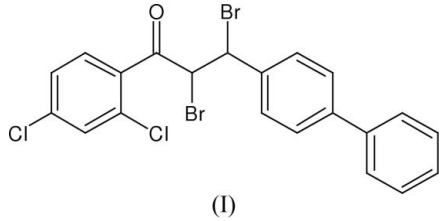
The two aromatic rings of the biphenyl group of the title compound, $C_{21}H_{14}Br_2Cl_2O$, are not coplanar and the carbonyl group is twisted out of the plane of the adjacent dichlorophenyl ring. The crystal packing is stabilized by C—H···O and C—H···Br contacts.

Comment

For a structurally simple group of compounds, chalcones display an impressive array of biological activities, among which antimalarial (Liu *et al.*, 2003), antiprotozoal (Nielson *et al.*, 1998), nitric oxide inhibition (Rajas *et al.*, 2002) and anticancer activities (Dinkova-Kostova *et al.*, 1998) have been reported in the literature. Among several organic compounds reported for non-linear optical (NLO) properties, chalcone derivatives are notable materials for their excellent blue light transmittance and good crystallizability. They provide a necessary configuration to show NLO properties, with two planar rings connected through a conjugated double bond (Goto *et al.*, 1991; Uchida *et al.*, 1998; Tam *et al.*, 1989; Indira *et al.*, 2002, Sarojini *et al.*, 2006).



(I)

The substitution of a bromo group on either of the phenyl rings greatly influences the non-centrosymmetric crystal packing. The bromo group can obviously improve the molecular first-order hyperpolarizabilities and can effectively reduce dipole–dipole interactions between the molecules. Chalcone derivatives usually have a lower melting temperature, which can be a drawback when we use these crystals in optical instruments. Chalcone dibromides usually have higher melting points and are thermally stable. Only a few structures of these compounds have been reported (Butcher, Yathirajan, Anilkumar *et al.*, 2006; Butcher, Yathirajan, Sarojini *et al.*, 2006; Harrison *et al.*, 2005). As a continuation of our studies on chalcones and their derivatives (Yathirajan *et al.*, 2006, and references therein), a chalcone dibromide, (I), was prepared by the bromination of chalcone [(2*E*)-3-(biphenyl-4-yl)-1-(2,4-dichlorophenyl)prop-2-en-1-one].

A perspective view of (I) is shown in Fig. 1. The two aromatic rings of the biphenyl residue are not coplanar [dihedral angle = 30.67 (9)°]. The carbonyl group is twisted out

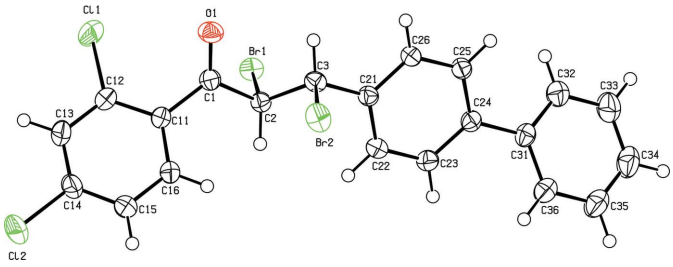


Figure 1
The molecular structure of the title compound, showing the atom numbering and displacement ellipsoids drawn at the 50% probability level.

of the plane of the adjacent dichlorophenyl ring (Table 1). The Br—C—C—Br unit adopts an almost perfect antiperiplanar conformation (Table 1). There are no classical hydrogen bonds, but the crystal packing is stabilized by C—H···O and C—H···Br contacts (Table 2).

Experimental

Chalcone [(2*E*)-3-(biphenyl-4-yl)-1-(2,4-dichlorophenyl)prop-2-en-1-one] (3.52 g, 0.01 mol) was treated with bromine in acetic acid (30%) until the orange colour of the solution persisted. After stirring for half an hour, the contents were poured on to crushed ice. The resulting solid mass was collected by filtration. The compound was dried and recrystallized from ethanol. Crystals suitable for a structure determination were obtained from an acetone and toluene (1:1) mixture by slow evaporation (yield 82%; m.p. 453–455 K). Analysis for $C_{21}H_{14}Br_2Cl_2O$ found (calculated): C 49.03 (49.16), H 2.69% (2.75%).

Crystal data

$C_{21}H_{14}Br_2Cl_2O$
M_r = 513.04
Monoclinic, $P2_1/c$
a = 18.1156 (9) Å
b = 11.1847 (5) Å
c = 9.9840 (5) Å
β = 100.762 (4)°
V = 1987.35 (17) Å^3
Z = 4
D_x = 1.715 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 4.36 mm^{-1}
T = 173 (2) K
Block, colourless
0.34 × 0.29 × 0.26 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.259, T_{max} = 0.335
29830 measured reflections
5863 independent reflections
5263 reflections with $I > 2\sigma(I)$
R_{int} = 0.057
θ_{max} = 30.2°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.091
S = 1.06
5863 reflections
236 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0395P)^2 + 2.0858P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.86 e Å^{-3}
$\Delta\rho_{min}$ = −1.26 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0083 (5)

Table 1
Selected torsion angles (°).

C1—C2—C3—C21	−174.25 (18)	O1—C1—C11—C12	41.0 (4)
Br1—C2—C3—Br2	179.19 (9)	O1—C1—C11—C16	−131.8 (3)

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15···O1^{i}	0.95	2.57	3.188 (3)	123
C16—H16···O1^{i}	0.95	2.60	3.211 (3)	123
C32—H32···O1^{ii}	0.95	2.54	3.482 (3)	172
C23—H23···Br1^{iii}	0.95	2.92	3.862 (2)	172

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

H atoms were found in a difference map, but they were refined using a riding model, with C—H = 0.95 Å for aromatic and C—H = 1.00 Å for tertiary H atoms. U_{iso}(H) values were set at 1.2U_{eq}(C). The deepest residual electron-density hole is located 0.69 Å from atom Br2.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON*.

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