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1,3-Bis(4-chlorophenyl)prop-2-en-1-one

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Key indicators

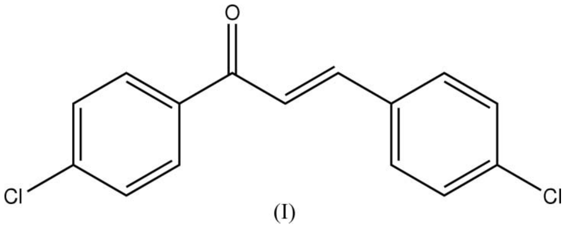
Single-crystal X-ray study
T = 193 K
Mean σ(C–C) = 0.003 Å
R factor = 0.048
wR factor = 0.105
Data-to-parameter ratio = 15.5

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

The non-planar title molecule, $C_{15}H_{10}Cl_2O$, contains two benzene rings linked by a –CH═CH–C(═O)– bridge. In the crystal structure, the molecules are paired through π–π interactions and the pairs are connected to each other via hydrogen-bonding interactions.

Comment

Chalcones with the general formula Ar–CH═CH–CO–Ar are an important class of compounds, with the common structural entity being the central –CH═CH–C(═O)– group, in which the H atoms can be substituted. The –C═C– double bond can be photoreactive and can produce various products through solid-state photocycloaddition. Therefore, chalcones are widely used in organic solid-state photochemistry (Satish *et al.*, 1995). In addition, with deliberate substitution, chalcones form a class of non-linear optical materials (Indira *et al.*, 2002). In these materials, the C═O bond acts as the electron-withdrawing group, and the electron-rich substituents in the aromatic rings serve as electron-donating groups, forming so-called *D*–π–*A* type molecules. When the electron-rich groups are located on the 4 and/or 4′ positions, the electron flow in the molecule follows a Λ-shaped path, and therefore the molecule is called a Λ-shaped molecule (Devia *et al.*, 1999). During our search for non-linear optical materials based on chalcones, the title compound, (I), was synthesized, and we present here the results of a study of the molecular packing in (I).



(I)

The molecule of (I) (Fig. 1 and Table 1) is not planar. The dihedral angles between the least-squares planes through atoms C1–C6 (plane 1), C7–C12 (plane 2) and C13–C15 (plane 3) are 46.0 (1) (planes 1 and 2), 11.9 (1) (planes 1 and 3) and 34.3 (1)° (planes 2 and 3). These data show that the benzene rings are rotated in opposite directions with respect to the central plane.

In the crystal structure of (I) (Fig. 2), the molecules are stacked through π–π interactions. The closest such interaction of 3.683 (2) Å occurs between the central –CH═CH–C(═O)– groups [symmetry operation (1 − *x*, 2 − *y*, −*z*)]. However, these are not perfectly aligned, so the shortest distance between the parallel C═C double bonds is

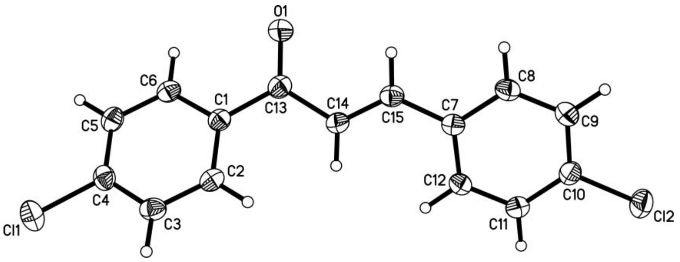


Figure 1
A view of (I), showing the atom-numbering scheme. Displacement ellipsoids are shown at the 40% probability level and H atoms are shown as small spheres of arbitrary radii.

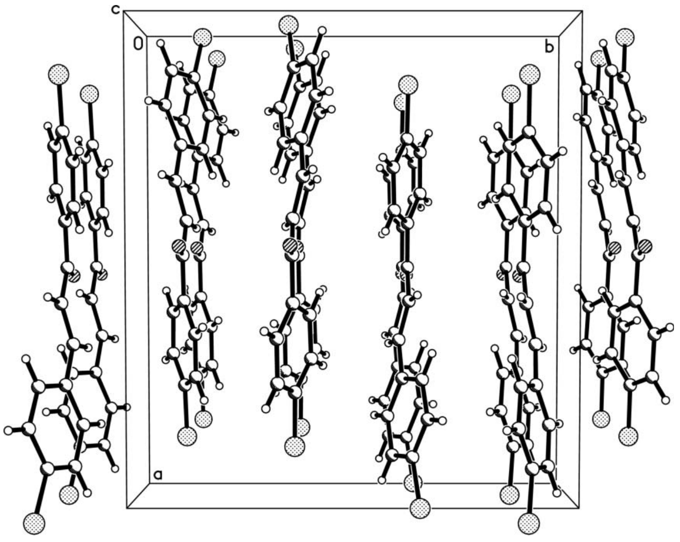


Figure 2
A packing diagram for (I), viewed down the *c* axis.

4.557 (2) Å, much longer than the reference value of 4.2 Å for a photoreactive crystal (Turowska-Tyrk *et al.*, 2003). The dihedral angle between the plane through the central group and that formed by the two C═C double bonds is 45.6 (1)°, also far from 90°, which is the perfect value for 2+2 photocycloaddition. These results are consistent with our observation that the molecule of (I) is stable, even after exposure to sunlight for 30 d and to an Hg lamp for 24 h.

An interesting feature in the structure of (I) is that pairs of molecules interact through three cooperative C—H⋯O hydrogen bonds (Desiraju, 2002). The phenone atom O1 is oriented so as to be located in the bay area defined by atoms H2, H12 and H14, and the C—H⋯O interactions (Table 2) serve to connect the pairs of molecules into a double chain. Additional interactions of the type C—H⋯Cl link the chains and there are also Cl⋯Cl interactions of note, with the closest contact of this type, 3.569 (1) Å, occurring between atoms Cl1 and Cl2^{ii} [symmetry code: (ii) −1 + *x*, *y*, −1 + *z*].

Experimental

The synthesis of the title compound (Migrdichian, 1957) was carried out by adding an aqueous solution of sodium hydroxide (10%, 10 ml) to a solution of 4-chloroacetophenone (0.02 mol) and 4-chlorobenzaldehyde (0.02 mol) in ethanol (95%, 30 ml). The reaction mixture was stirred at room temperature for 4 h and then neutralized with HCl (10%) and water. The product was recrystallized three times from ethanol (95%). Colourless crystals were obtained by slow evaporation (over 10 d) of a solution of (I) in absolute ethanol at 293 K (m.p. 428–430 K). Elemental analysis (Perkin–Elmer 240C elemental analyzer): calculated for $C_{15}H_{10}Cl_2O$: C 64.98, H 3.61; found: C 64.81, H 3.86%. IR (FT–IR spectrophotometer with KBr pellets, ν, cm^{-1}): 1657 (*s*, C═O), 1605 (*s*, –CH═CH–), 1588 (*s*), 1563 (*s*, pH), 1490 (*s*), 1405 (*m*), 1332 (*s*), 1220 (*s*), 1099 (*s*), 818 (*s*), 800 (*m*), 743 (*m*), 666 (*m*).

Crystal data

$C_{15}H_{10}Cl_2O$
$M_r = 277.13$
Monoclinic, $P2_1/c$
$a = 15.325$ (3) Å
$b = 14.009$ (2) Å
$c = 5.8501$ (10) Å
$\beta = 92.908$ (4)°
$V = 1254.3$ (4) Å^3
$Z = 4$

$D_x = 1.468$ Mg m^{-3}
Mo *K*α radiation
Cell parameters from 4017 reflections
$\theta = 3.0$–26.4°
$\mu = 0.50$ mm^{-1}
$T = 193$ (2) K
Block, colourless
0.25 × 0.23 × 0.10 mm

Data collection

Rigaku Mercury diffractometer
ω and φ scans
Absorption correction: multi-scan (*ABSCOR*; Jacobson, 1998)
$T_{min} = 0.885$, $T_{max} = 0.952$
12957 measured reflections
2549 independent reflections

2109 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$
$\theta_{max} = 26.4$°
$h = -19 \rightarrow 19$
$k = -17 \rightarrow 16$
$l = -7 \rightarrow 7$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.105$
$S = 1.15$
2549 reflections
164 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 0.6039P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.25$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cl1—C4	1.737 (2)	C7—C15	1.458 (3)
Cl2—C10	1.735 (2)	C13—C14	1.479 (3)
O1—C13	1.231 (3)	C14—C15	1.326 (3)
C1—C13	1.490 (3)		
C6—C1—C2	118.8 (2)	C9—C10—C11	121.2 (2)
C6—C1—C13	119.05 (19)	C9—C10—Cl2	120.17 (17)
C2—C1—C13	122.11 (19)	C11—C10—Cl2	118.67 (17)
C3—C4—C5	121.7 (2)	O1—C13—C14	121.2 (2)
C3—C4—Cl1	119.00 (17)	O1—C13—C1	119.9 (2)
C5—C4—Cl1	119.31 (17)	C14—C13—C1	118.95 (18)
C8—C7—C12	117.96 (19)	C15—C14—C13	121.34 (19)
C8—C7—C15	119.53 (18)	C14—C15—C7	127.33 (19)
C12—C7—C15	122.44 (19)		
C13—C1—C2—C3	177.48 (19)	C2—C1—C13—O1	−157.7 (2)
C2—C3—C4—Cl1	176.91 (16)	C6—C1—C13—C14	−158.45 (19)
Cl1—C4—C5—C6	−178.24 (16)	C2—C1—C13—C14	23.2 (3)
C13—C1—C6—C5	−178.89 (19)	O1—C13—C14—C15	17.3 (3)
C15—C7—C8—C9	−176.1 (2)	C1—C13—C14—C15	−163.6 (2)
C8—C9—C10—Cl2	179.14 (17)	C13—C14—C15—C7	−174.3 (2)
Cl2—C10—C11—C12	−179.68 (16)	C8—C7—C15—C14	−176.1 (2)
C15—C7—C12—C11	175.48 (19)	C12—C7—C15—C14	6.9 (3)
C6—C1—C13—O1	20.7 (3)		

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2···O1^{i}	0.95	2.81	3.613 (3)	143
C14—H14···O1^{i}	0.95	2.81	3.719 (3)	160
C12—H12···O1^{i}	0.95	2.84	3.680 (3)	148
C9—H9···Cl1^{ii}	0.95	3.02	3.825 (2)	144

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

H atoms were included in the riding-model approximation, with C—H distances set at 0.95 Å and with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(carrier atom).

Data collection: *CrystalClear* (Rigaku, 1999); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku, 2000); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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