Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Chlorophenyl)-1-(2,4-dichlorophenyl)-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 = 0.049
wR factor = 0.137
Data-to-parameter ratio = 35.7

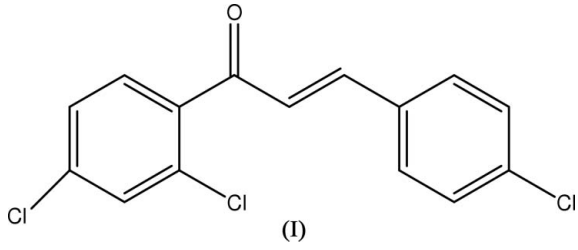
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 March 2006
Accepted 11 March 2006

In the title compound, $C_{15}H_9Cl_{13}O$, the enone unit and the benzene rings are each planar. The molecules are linked *via* weak C—H···Cl interactions into wave-like chains along the *a* axis and are stacked parallel to the *b* axis.

Comment

Among many organic compounds reported for their second harmonic generation, chalcone derivatives have attracted much interest as they exhibit extremely high and fast non-linearity (Fichou *et al.*, 1988; Patil *et al.*, 2006; Uchida *et al.*, 1998), much better than that observed in inorganic crystals. In this paper, we report the structure of the title compound, (I). These crystals do not exhibit second-order NLO properties as they crystallize in a centrosymmetric space group.



(I)

The bond lengths and angles are within normal ranges (Allen *et al.*, 1987) and compare well with those reported in other related structures (Jeyabharathi *et al.*, 2002; Ng *et al.*, 2006*a*,*b*; Patil *et al.*, 2006; Ravishankar *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Radhika *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Santhi & Fun, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Selvam *et al.*, 2005; Sathiya Moorthi, Chinnakali, Nanjundan, Unnithan *et al.*, 2005; Teh *et al.*, 2006). The short Cl2···H8*A* (2.82 Å) contact causes the bond angles C5—C6—C7 [124.82 (14)°] and C6—C7—C8 [117.73 (14)°] to deviate significantly from 120°. Furthermore, the short H8*A*···H11*A* (2.19 Å) contact results in widening of the C9—C10—C11 angle to 122.02 (15)°.

The enone unit O1/C7–C9 and the two benzene rings C1–C6 and C10–C15 of the chalcone are each planar, with maximum deviations of 0.050 (2), 0.009 (2) and 0.004 (2) Å for atoms C7, C6 and C15, respectively. The molecule is slightly twisted about the C6—C7 bond; relevant torsion angles are C1—C6–C7—C8 = −134.30 (17)°, C6—C7—C8—C9 = −169.94 (17)°, C7—C8—C9—C10 = 178.00 (17)° and C8—C9—C10—C15 = 170.03 (18)°. The dihedral angle between the two benzene rings is 41.99 (5)°. The least-squares plane through the enone unit makes dihedral angles of 44.81 (6) and 5.91 (8)° with the C1–C6 and C10–C15 benzene rings, respectively.

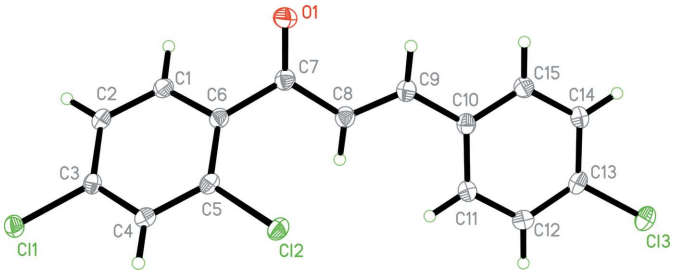


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering.

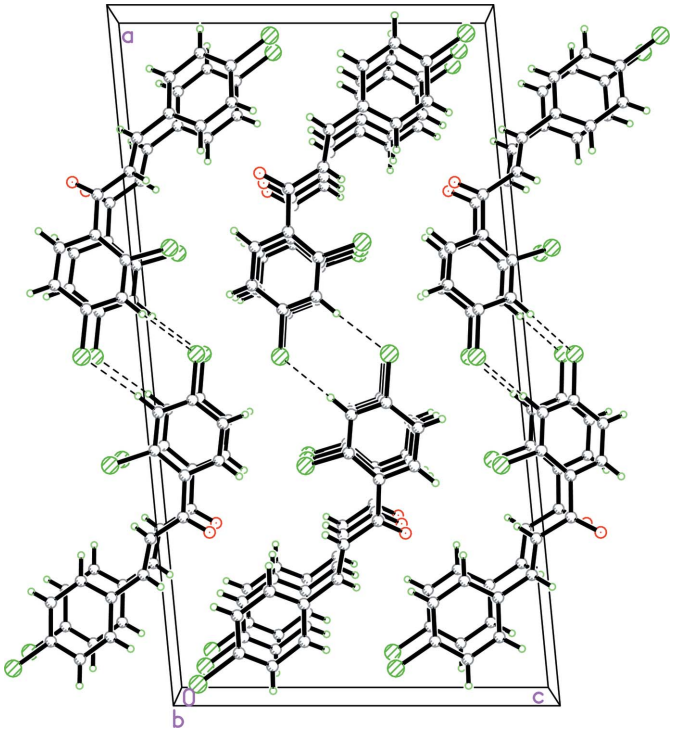


Figure 2
The crystal packing of (I), viewed down the *b* axis. Intermolecular C—H···Cl interactions are shown as dashed lines.

A very weak intermolecular C—H···Cl interaction is observed in the crystal structure between atoms C4 and Cl1 [C4—H4*A* = 0.93 Å, C4···Cl1 = 3.706 (2) Å, H4*A*···Cl1 = 2.87 Å and C4—H4*A*···Cl1 = 151°]. These weak interactions link the molecules, forming wave-like infinite chains along the *a* axis. These chains are stacked parallel to the *b* axis.

Experimental

Commercially available AR grade 4-chlorobenzaldehyde, 2,4-dichloroacetophenone and ethanol (99%) were used without further purification to synthesize the title chalcone derivative, (I), by adapting the Claisen–Schmidt condensation reaction (Dhar, 1981). 4-Chlorobenzaldehyde (0.01 mol) in ethanol (30 ml) and 4-dichloroaceptophenone (0.01 mol) in ethanol (30 ml) were mixed together, and the mixture was treated with an aqueous solution of NaOH (3 ml, 30%). After stirring for 3 h, the contents of the flask were poured into ice-cold water (250 ml). The resulting crude solid was collected by filtration. The compound was dried and purified by repeated recrystallization from acetone. The purity of the compound was checked by thin layer chromatography. Crystals of (I) suitable for a single-crystal X-ray diffraction study were grown over a period of 12 d by slow evaporation of an acetone solution.

Crystal data

$C_{15}H_9Cl_3O$
M_r = 311.57
Monoclinic, $P2_1/c$
a = 24.9624 (7) Å
b = 3.8201 (1) Å
c = 13.7230 (4) Å
β = 95.430 (1)°
V = 1302.74 (6) Å^3
Z = 4
D_x = 1.589 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 5105 reflections
θ = 0.8–35.9°
μ = 0.69 mm^{-1}
T = 100.0 (1) K
Block, colourless
0.32 × 0.15 × 0.15 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.777, T_{max} = 0.906
26316 measured reflections
6146 independent reflections
4428 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
θ_{max} = 35.9°
$h = -41 \rightarrow 41$
$k = -6 \rightarrow 6$
$l = -22 \rightarrow 21$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.137
S = 1.07
6146 reflections
172 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0635P)^2 + 0.5011P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.48 e Å^{-3}
$\Delta\rho_{min}$ = −0.64 e Å^{-3}

H atoms were placed in calculated positions and refined as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(carrier atom).

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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government and Universiti Sains Malaysia for the Scientific Advancement Grant Allocation (SAGA) grant No. 304/PFIZIK/653003/A118 and the short-term grant No. 304/PFIZIK/635028.

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