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1,5-Bis(4-chlorophenyl)penta-1,4-dien-3-one

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Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.007 Å
R factor = 0.079
wR factor = 0.245
Data-to-parameter ratio = 22.4

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

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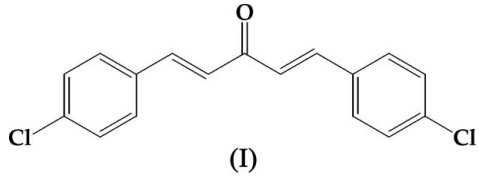
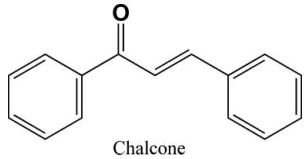
The title compound, $C_{17}H_{12}Cl_2O$, shows significant non-linear optical activity. A twofold rotation axis passes through the carbonyl group.

Comment

The title compound, (I), crystallizes in the non-centrosymmetric space group $P2_12_12$ and shows significant nonlinear optical (NLO) activity. Among several organic compounds exhibiting NLO activity, chalcone derivatives (see second scheme below) are of interest owing to their excellent blue light transmittance and ease of crystallization. They provide a necessary configuration for NLO activity, with two planar rings connected through a conjugated double bond (Indira *et al.*, 2002). They are also inherently chiral owing to the fact that the two phenyl rings are mutually twisted with respect to the linking backbone (Butcher, Yathirajan, Sarojini *et al.*, 2006; Butcher *et al.*, 2006*a*,*b*). This helicity has also been shown to lead to NLO activity (Botek *et al.*, 2004; Daul *et al.*, 2003; Verbiest *et al.*, 1998). Bis-chalcones are also found to exhibit good NLO properties (Uchida *et al.*, 1998).



(I)



Chalcone

In view of the importance of chalcones (Butcher, Yathirajan, Sarojini *et al.*, 2006; Butcher *et al.*, 2006*a*,*b*), the present paper reports the crystal structure of (I), a bis-chalcone derivative. As indicated above, this compound also crystallizes in a chiral space group, $P2_12_12$, despite the absence of a chiral center. This chirality arises from the fact that the molecule is twisted so that the two benzene rings are not coplanar [dihedral angle 53.4 (5)°]. A twofold rotation axis passes through C1 and O1. The five-C-atom backbone shows alternating double and single bonds [C1—C2 = 1.579 (10) Å, C2═C3 = 1.239 (7) Å and C3—C4 =1.502 (7) Å] and thus gives no indication of conjugation. The most commonly cited factors found in organic molecules possessing NLO properties are the presence of donor–acceptor substituents on a conju-

gated backbone. Since this molecule does not possess either of these factors the helicity of the molecule must be the origin of the observed NLO effects.

Experimental

The title compound was synthesized according to the reported method (Furnis *et al.*, 1989) with a yield of 80%. The compound was purified by recrystallization from ethanol. Crystals were grown from acetone/toluene (1:1) by slow evaporation. The second harmonic generation efficiency of this compound, normalized to that of urea, was measured by the standard powder technique (Kurtz & Perry, 1968) using an Nd:YAG laser and found to be 5.0 times that of urea. M.p. 383 K; yield 80%. Analysis calculated C 67.35, H 3.99%; found C 67.17, H 3.76%.

Crystal data

$C_{17}H_{12}Cl_2O$
M_r = 303.17
Orthorhombic, $P2_12_12$
a = 24.509 (3) Å
b = 4.9846 (5) Å
c = 5.8103 (6) Å
V = 709.82 (13) Å^3
Z = 2
D_x = 1.418 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.45 mm^{-1}
T = 298 (2) K
Chunk, colorless
0.38 × 0.36 × 0.28 mm

Data collection

Bruker APEX2 CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.848, T_{max} = 0.885
7671 measured reflections
2063 independent reflections
1630 reflections with $I > 2\sigma(I)$
R_{int} = 0.026
θ_{max} = 30.7°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.245
S = 1.07
2063 reflections
92 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1266P)^2 + 0.4423P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.015
$\Delta\rho_{max}$ = 0.69 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}
Absolute structure: Flack (1983), 739 Friedel pairs
Flack parameter: 0.2 (2)

Table 1
Selected geometric parameters (Å, °).

Cl—C7	1.747 (4)	C2—C3	1.239 (7)
O—C1	1.170 (12)	C3—C4	1.502 (7)
C1—C2	1.579 (10)	C4—C9	1.371 (7)
O—C1—C2	128.5 (4)	C3—C2—C1	119.8 (7)
C2—C1—C2^{i}	103.1 (9)	C2—C3—C4	124.0 (6)

Symmetry code: (i) $-x+1, -y+2, z$.

All H atoms were initially located in a difference Fourier map. All H atoms were then placed in geometrically idealized positions and constrained to ride on their parent atoms with C—H distances of 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *APEX2*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

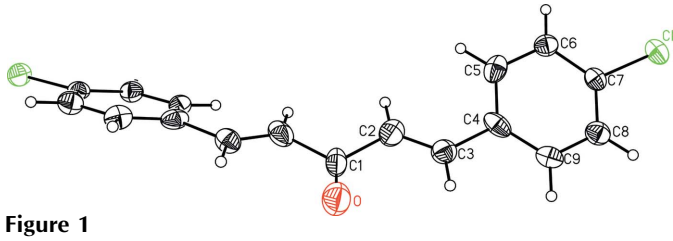


Figure 1
View of (I), showing the atom-numbering scheme. Unlabelled atoms are related to labelled atoms by the symmetry code $(1-x, 2-y, z)$.

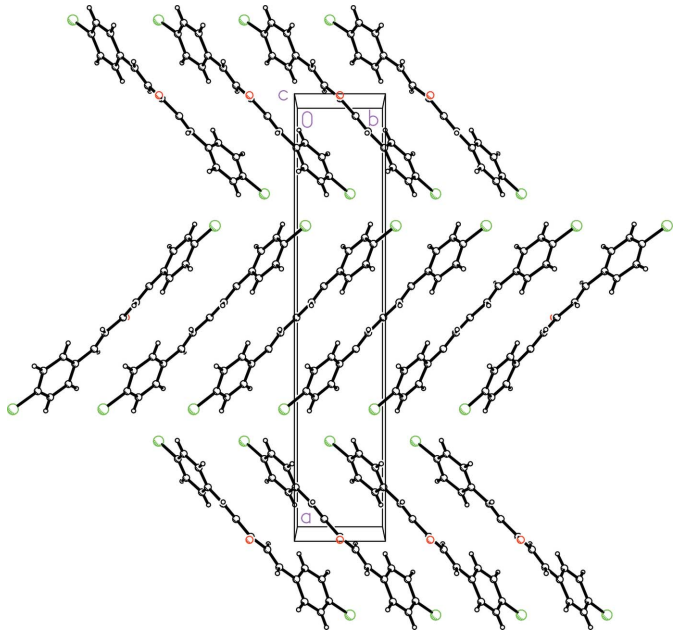


Figure 2
The molecular packing of (I), viewed down the *c* axis.

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References

Botek, E., Champagne, B., Turki, M. & André, J.-M. (2004). *J. Chem. Phys.* **120**, 2042–2048.
Bruker (2006). *APEX2*. Version 2.0-2. Bruker AXS Inc., Madison Wisconsin, USA.
Butcher, R. J., Yathirajan, H. S., Anilkumar, H. G., Sarojini, B. K. & Narayana, B. (2006*a*). *Acta Cryst.* E**62**, o1633–o1635.
Butcher, R. J., Yathirajan, H. S., Anilkumar, H. G., Sarojini, B. K. & Narayana, B. (2006*b*). *Acta Cryst.* E**62**, o1659–o1661.
Butcher, R. J., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Mithun, A. (2006). *Acta Cryst.* E**62**, o1629–o1630.
Daul, C. A., Ciofini, I. & Weber, V. (2003). *Int. J. Quantum Chem.* **91**, 297–302.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Furnis, B. S., Hannaford, A. J., Smith, P. W. G. & Tatchell, A. R. (1989). *Vogel's Textbook of Practical Organic Chemistry*, 5th ed., p. 1033. New York: Longman Group UK Ltd.
Indira, J., Karat, P. P. & Sarojini, B. K. (2002). *J. Cryst. Growth*, **242**, 209–214.
Kurtz, S. K. & Perry, T. T. (1968). *J. Appl. Phys.* **39**, 3798–3813.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*a*). *SHELXL97*. University of Göttingen, Germany.
Sheldrick, G. M. (1997*b*). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.

Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abduryim, A. & Watanabe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **315**, 135–140.

Verbiest, T., Van Elschocht, S., Kauranen, M., Hellemans, L., Snauwaert, J., Nuckolls, C., Katz, T. J. & Persoons, A. (1998). *Science*, **282**, 913–915.