Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

(2*E*)-1-(2,4-Dichlorophenyl)-3-(4-nitrophenyl)-prop-2-en-1-one

H. S. Yathirajan,[a] A. N. Mayekar,[a] B. K. Sarojini,[b] B. Narayana[b] and Michael Bolte[c]*

[a]Department of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, [b]Department of Chemistry, Mangalore University, Mangalagangotri 574 199, India, and [c]Institut für Anorganische Chemie, J. W. Goethe-Universität Frankfurt, Max-von-Laue-Strasse 7, 60438 Frankfurt/Main, Germany

Correspondence e-mail: bolte@chemie.uni-frankfurt.de

Key indicators

Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.005 Å
R factor = 0.037
wR factor = 0.093
Data-to-parameter ratio = 12.1

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

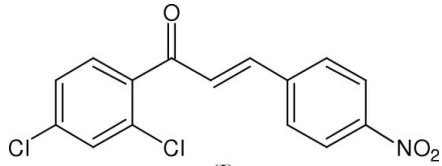
© 2007 International Union of Crystallography
All rights reserved

Received 18 December 2006
Accepted 18 December 2006

In the title compound, $C_{15}H_9Cl_2NO_3$, the central double bond is *trans* configured and the dihedral angle between the two planar fragments of the molecule is 44.53 (4)°. The crystal packing is stabilized by C—H···O and C—H···Cl contacts.

Comment

In continuation of our work on chalcones (Yathirajan *et al.*, 2006) as possible non-linear optical hosts (Sarojini *et al.*, 2006), the present paper reports the crystal structure of a newly synthesized chalcone, (I) (Fig. 1). The crystal structures of some other dichloro-substituted chalcones have been reported recently (Teh *et al.*, 2006; Ng *et al.*, 2006). We have previously described the crystal structures of 1-(2,4-dichloro-5-fluorophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (Yathirajan *et al.*, 2006) and (2E)-1-(2,4-dichlorophenyl)-3-[4-(methylsulfanyl) phenyl]prop-2-en-1-one (Butcher *et al.*, 2007).



(I)

The bond lengths and angles in (I) can be regarded as normal (Cambridge Structural Database, Version 5.27, November 2005, updated August 2006; *MOGUL* Version 1.1; Allen, 2002). The central double bond is *trans* configured and the O1—C1—C2—C3 torsion angle is −7.5 (5)°. The nitro group is almost coplanar with the aromatic ring to which it is attached. Thus, the molecule consists of two essentially planar moieties, one of which is the dichlorophenyl ring (r.m.s. deviation = 0.015 Å) while the other consists of the remaining non-H atoms (r.m.s. deviation = 0.059 Å). The dihedral angle between these mean planes is 44.53 (4)°.

The crystal packing of (I) is stabilized by C—H···O and C—H···Cl contacts (Table 1).

Experimental

2,4-Dichloroacetophenone (1.89 g, 0.01 mol) in methanol (25 ml) was mixed with 4-nitrobenzaldehyde (1.51 g, 0.01 mol) and the mixture was treated with 30% potassium hydroxide solution (4 ml) at 278 K. The reaction mixture was then brought to room temperature and stirred for 10 h. The precipitated solids were filtered and washed with water, dried and recrystallized from an acetone–toluene (1:1 *v*/*v*) mixture (m.p. 427–429 K). Analysis for $C_{15}H_9Cl_2NO_3$: found (calculated): C 55.83 (55.93), H 2.76 (2.82), N 4.24 (4.35)%.

Crystal data

$C_{15}H_9Cl_2NO_3$
M_r = 322.13
Monoclinic, $P2_1$
a = 3.7973 (5) Å
b = 7.1528 (9) Å
c = 25.336 (3) Å
β = 90.386 (11)°
V = 688.14 (15) Å^3
Z = 2
D_x = 1.555 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.48 mm^{-1}
T = 173 (2) K
Plate, light yellow
0.22 × 0.18 × 0.09 mm

Data collection

Stoe IPDS-II two-circle diffractometer
ω scans
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.892, T_{max} = 0.948
3300 measured reflections
2313 independent reflections
2046 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.1°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
S = 1.00
2313 reflections
191 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 1997)
Extinction coefficient: 0.049 (5)
Absolute structure: Flack (1983), with 994 Friedel pairs
Flack parameter: −0.03 (8)

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C13—H13···Cl2^{i}	0.95	2.83	3.678 (3)	149
C22—H22···O11^{ii}	0.95	2.58	3.455 (4)	153
C23—H23···O12^{iii}	0.95	2.51	3.216 (4)	131
C25—H25···O1^{iv}	0.95	2.46	3.255 (4)	141

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

The H atoms were found in a difference map, repositioned in idealized locations with C—H = 0.95 Å, and refined as riding, with $U_{iso}(H) = 1.2U_{eq}(C)$.

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*.

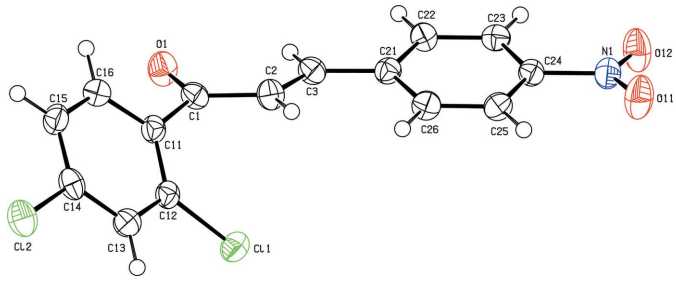


Figure 1
A view of the molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

ANM thanks the University of Mysore for permission to carry out this research work. BKS thanks AICTE, Government of India, for financial assistance through the Career Award for Young Teachers Scheme.

References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Butcher, R. J., Yathirajan, H. S., Narayana, B., Mithun, A. & Sarojini, B. K. (2007). *Acta Cryst.* E**63**, o30–o32.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Ng, S.-L., Razak, I. A., Fun, H.-K., Patil, P. S. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o4653–o4655.
Sarojini, B. K., Narayana, B., Ashalatha, B. V., Indira, J. & Lobo, K. J. (2006). *J. Cryst. Growth*, **295**, 54–59.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (2001). *X-AREA*. Stoe & Cie, Darmstadt, Germany.
Teh, J. B.-J., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprakash, S. M. (2006). *Acta Cryst.* E**62**, o4380–o4381.
Yathirajan, H. S., Sarojini, B. K., Narayana, B., Bindya, S. & Bolte, M. (2006). *Acta Cryst.* E**62**, o3631–o3632.