

William T. A. Harrison,^{a*}
 H. S. Yathirajan,^b B. Narayana,^c
 T. V. Sreevidya^c and K. Sunil^c

^aDepartment of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland, ^bDepartment of Studies in Chemistry, University of Mysore, Manasagangotri, Mysore 570 006, India, and ^cDepartment of Chemistry, Mangalore University, Mangalagangotri 574 199, India

Correspondence e-mail:
 w.harrison@abdn.ac.uk

Key indicators

Single-crystal X-ray study
 T = 120 K
 Mean $\sigma(\text{C}-\text{C}) = 0.004 \text{ \AA}$
 R factor = 0.027
 wR factor = 0.058
 Data-to-parameter ratio = 15.7

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

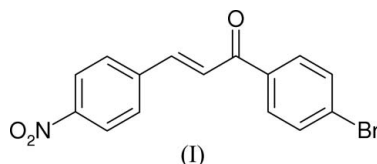
(2E)-1-(4-Bromophenyl)-3-(4-nitrophenyl)-prop-2-en-1-one

In the approximately planar molecule of the title compound, $\text{C}_{15}\text{H}_{10}\text{BrNO}_3$, the dihedral angle between the two benzene rings is $4.97 (18)^\circ$. Intermolecular $\text{C}-\text{H} \cdots \text{O}$ interactions help to form chains of molecules in the crystal structure.

Received 18 September 2006
 Accepted 28 September 2006

Comment

Chalcone derivatives show considerable promise as organic non-linear optical materials (Uchida *et al.*, 1998). As part of our ongoing studies of these compounds (Harrison *et al.*, 2006), the synthesis and structure of the title compound, (I) (Fig. 1), is presented here. Compound (I) is an isomer of the recently reported 3-(4-bromophenyl)-1-(4-nitrophenyl)prop-2-en-1-one [(II); Rosli *et al.*, 2006], in which the bromo and nitro substituents are exchanged on the benzene rings.



The geometrical parameters for (I) fall within their expected ranges (Allen *et al.*, 1987). The degree of twisting about the C_6-C_7 and C_9-C_{10} bonds in (I) (Table 1) is almost the same, but in opposite senses. This results in the C_1-C_6 and $\text{C}_{10}-\text{C}_{15}$ benzene-ring mean planes in (I) being close to parallel [dihedral angle = $4.97 (18)^\circ$]. By comparison, in compound (II), the dihedral angles between the mean planes of the corresponding benzene rings in the two molecules of the asymmetric unit are $12.83 (7)$ and $41.15 (7)^\circ$. The well ordered nitro group in (I) is slightly twisted away from the $\text{C}_{10}-\text{C}_{15}$ benzene ring mean plane [dihedral angle = $3.4 (4)^\circ$].

A PLATON (Spek, 2003) analysis of (I) indicated two possible intermolecular $\text{C}-\text{H} \cdots \text{O}$ interactions (Table 2) that result in chains of molecules (Fig. 2) propagating in either

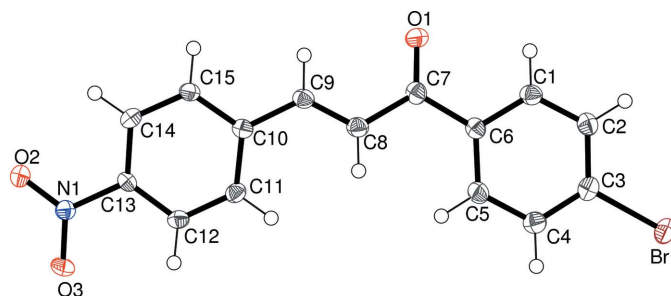
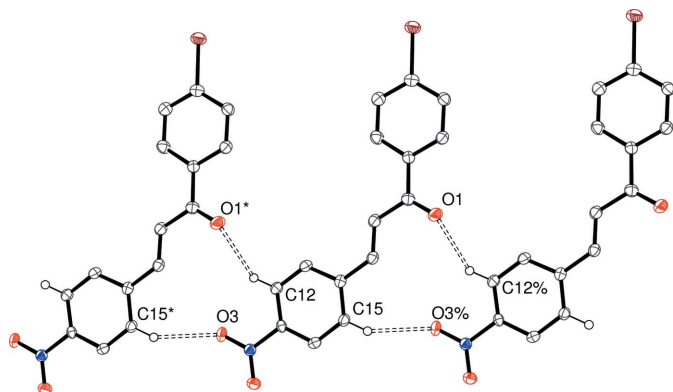


Figure 1
 View of the molecular structure of (I) showing 50% probability displacement ellipsoids.


Figure 2

Detail of (I), showing the C—H...O interactions (dashed lines) that link the molecules into [011] and $[0\bar{1}1]$ chains. Atoms with the suffixes * and % are generated by the symmetry operations $(x, y - 1, z + 1)$ and $(x, y + 1, z - 1)$, respectively.

[011] or $[0\bar{1}1]$. The graph-theory (Bernstein *et al.*, 1995) notation for the closed loop that results is $R_2^2(12)$. Overall, the packing (Fig. 3) results in zigzag (100) sheets of (I). The packing in (II) is completely different: all molecules are aligned in approximately the same orientation, resulting in a layered structure in the centrosymmetric space group $P\bar{1}$.

Experimental

A solution of potassium hydroxide (5%, 5 ml) was added slowly with stirring to a mixture of 4-nitrobenzaldehyde (1.51 g, 0.01 mol) and 4-bromoacetophenone (1.99 g, 0.01 mol) in ethanol (30 ml). The mixture was stirred at room temperature for 24 h. The precipitated solid was filtered, washed with water, dried and crystals of (I) were recrystallized from acetone by slow evaporation (yield: 68%; m.p. 439–441 K). Analysis found (calculated) for $C_{15}H_{10}BrNO_3$ (%): C 54.11 (54.24), H 3.04 (3.03), N 4.10 (4.22).

Crystal data

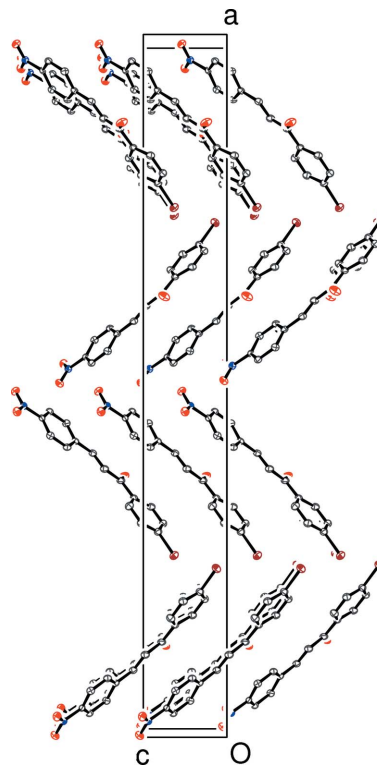
$C_{15}H_{10}BrNO_3$	$Z = 4$
$M_r = 332.15$	$D_x = 1.679 \text{ Mg m}^{-3}$
Orthorhombic, $Pna2_1$	Mo $K\alpha$ radiation
$a = 43.007(3) \text{ \AA}$	$\mu = 3.13 \text{ mm}^{-1}$
$b = 5.9744(4) \text{ \AA}$	$T = 120(2) \text{ K}$
$c = 5.1137(3) \text{ \AA}$	Slab, light yellow
$V = 1313.92(15) \text{ \AA}^3$	$0.48 \times 0.34 \times 0.16 \text{ mm}$

Data collection

Nonius KappaCCD diffractometer	9881 measured reflections
ω and φ scans	2833 independent reflections
Absorption correction: multi-scan	2452 reflections with $I > 2\sigma(I)$
(SADABS; Bruker, 2003)	$R_{\text{int}} = 0.034$
$T_{\text{min}} = 0.315$, $T_{\text{max}} = 0.634$	$\theta_{\text{max}} = 27.6^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0103P)^2 + 0.5147P]$
$R[F^2 > 2\sigma(F^2)] = 0.027$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.058$	$(\Delta/\sigma)_{\text{max}} = 0.001$
$S = 1.02$	$\Delta\rho_{\text{max}} = 0.42 \text{ e \AA}^{-3}$
2833 reflections	$\Delta\rho_{\text{min}} = -0.37 \text{ e \AA}^{-3}$
181 parameters	Absolute structure: Flack (1983),
H-atom parameters constrained	1143 Friedel pairs
	Flack parameter: 0.039 (9)


Figure 3

The unit cell contents of (I), viewed down [010]. H atoms have been omitted.

Table 1

Selected torsion angles ($^\circ$).

C1—C6—C7—O1	9.1 (4)	C8—C9—C10—C11	−9.3 (5)
-------------	---------	---------------	----------

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C12—H12...O1 ⁱ	0.95	2.51	3.218 (3)	131
C15—H15...O3 ⁱⁱ	0.95	2.46	3.296 (3)	146

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

The H atoms were positioned geometrically ($C-H = 0.95 \text{ \AA}$) and refined as riding, with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{carrier})$.

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997), and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

We thank the EPSRC National Crystallography Service (University of Southampton) for the data collection. BKS thanks AICTE, Government of India, New Delhi, for financial assistance under the 'Career Award for Young Teachers' scheme.

References

- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bernstein, J., Davies, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
- Blessing, R. H. (1995). *Acta Cryst.* **A51**, 33–38.
- Bruker (2003). *SADABS*, Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.
- Harrison, W. T. A., Yathirajan, H. S., Sarojini, B. K., Narayana, B. & Vijaya Raj, K. K. (2006). *Acta Cryst.* **E62**, o1578–o1579.
- Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography, Part A*, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Rosli, M. M., Patil, P. S., Fun, H.-K., Razak, I. A. & Dharmaprasanth, S. M. (2006). *Acta Cryst.* **E62**, o1466–o1468.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Uchida, T., Kozawa, K., Sakai, T., Aoki, M., Yoguchi, H., Abduryim, A. & Watanabe, Y. (1998). *Mol. Cryst. Liq. Cryst.* **315**, 135–140.