organic papers

3-(4-Bromophenyl)-1-(4-nitrophenyl)-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 = 0.032
wR factor = 0.085
Data-to-parameter ratio = 30.7

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

In the title compound, $C_{15}H_{10}BrNO_3$, the molecules are
arranged into infinite chains through Br···O short inter-
actions. The chains are stacked to form layers. These layers are
interconnected by C—H···O interactions. There are two
molecules in the asymmetric unit.

Comment

Chalcones have been claimed to be a class of compounds that
play a vital role in antitumour (Mishra *et al.*, 2001), anti-
inflammatory (Ko *et al.*, 2003; Tuchinda *et al.*, 2002) and
antimalarial (Domínguez *et al.*, 2001) activities. It has also
been documented that chalcones exhibit extremely high and
fast non-linearity (Fichou *et al.*, 1988; Zhang *et al.*, 1990; Zhao
et al., 2000) and are easy to crystallize as non-centrosymmetric
structures. Another importance of this type of compounds is
their high photosensitivity and thermal stability, which are
used in developing various crystalline electro-optical devices
(Williams *et al.*, 1983; Chemla *et al.*,1987). In view of their
exceptional behaviour, chalcones have been the subject of
several experimental and theoretical studies, aimed mainly at
determining their crystal structures (Moorthi *et al.*, 2005;
Radha Krishna *et al.*, 2005; Uchida *et al.*, 1995). In this work,
we report the synthesis and crystal structure of 3-(4-bromo-
phenyl)-1-(4-nitrophenyl)prop-2-en-1-one, (I).

(I)
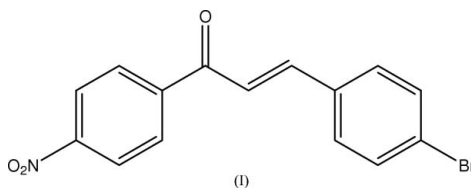
There are two molecules in the asymmetric unit of (I). The
bond parameters are comparable with those in related struc-
tures (Teh *et al.*, 2006; Ng *et al.*, 2006; Patil *et al.*, 2006). The
dihedral angle between the benzene rings is 12.83 (7)° for
molecule *A* and 41.15 (7)° for molecule *B*. The nitro group
attached at C13 is twisted away from the C10–C15 benzene
ring, with torsion angles O2—N1—C13—C14 = −5.8 (2) and
12.2 (2)°, and O3—N1—C13—C12 = −6.0 (2) and 12.9 (2)° for
molecules *A* and *B*, repectively. The least-squares plane
through the enone fragment makes dihedral angles of
16.36 (6) and 17.09 (6)° with the C1–C6 and C10–C15 benzene
rings for molecule *A*, and of 24.49 (11) and 18.56 (12)° for
molecule *B*.

In the crystal structure of (I), the intramolecular C7—
H7*A*···O1 interaction generates an *S*(5) ring motif (Bernstein
et al., 1995) for both molecules *A* and *B*. The molecules are

arranged into infinite chains through short Br1A···O2B(−1 + x, 1 + y, z) [3.0417 (14) Å] interactions and also weak short Br1A···O3B(x, 1 + y, z) [3.3741 (13) Å] interactions. These chains are stacked to form layers which are interconnected by C—H···O interactions (Table 1).

Experimental

Chalcone derivative (I) was obtained by the condensation of 4-bromobenzaldehyde (0.01 mol) and 4′-nitroacetophenone (0.01 mol) in ethanol (60 ml) in the presence of NaOH (2 ml, 30%). The resulting crude solid compound was collected by filtration, dried and recrystallized from acetone. Crystals suitable for X-ray diffraction study were grown by slow evaporation of an acetone solution over a period of 7 d.

Crystal data

C$_{15}$H$_{10}$BrNO$_3$	$Z = 4$
$M_r = 332.15$	$D_x = 1.740$ Mg m^{-3}
Triclinic, $P\bar{1}$	Mo $K\alpha$ radiation
$a = 5.9341$ (1) Å	Cell parameters from 6533
$b = 7.9193$ (1) Å	reflections
$c = 27.2996$ (4) Å	$\theta = 0.8$–$35.0°$
$\alpha = 89.938$ (1)°	$\mu = 3.25$ mm^{-1}
$\beta = 85.622$ (1)°	$T = 100.0$ (1) K
$\gamma = 82.357$ (1)°	Block, yellow
$V = 1267.75$ (3) Å^3	$0.55 \times 0.39 \times 0.25$ mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	11069 independent reflections
	9020 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.036$
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)	$\theta_{max} = 35.0°$
	$h = -9 \rightarrow 9$
$T_{min} = 0.286$, $T_{max} = 0.444$	$k = -12 \rightarrow 12$
41078 measured reflections	$l = -44 \rightarrow 39$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0409P)^2$
$R[F^2 > 2\sigma(F^2)] = 0.033$	$+ 0.3692P]$
$wR(F^2) = 0.085$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{max} = 0.002$
11069 reflections	$\Delta\rho_{max} = 0.94$ e Å^{-3}
361 parameters	$\Delta\rho_{min} = -0.57$ e Å^{-3}
H-atom parameters constrained	

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

D—H···A	D—H	H···A	D···A	D—H···A
C7A—H7AA···O1A	0.93	2.46	2.804 (2)	102
C7B—H7BA···O1B	0.93	2.49	2.812 (2)	100
C15B—H15B···O1A^i	0.93	2.58	3.240 (2)	129

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

H atoms were placed in calculated positions, with C—H distances of 0.93 Å. The U_{iso}(H) values were constrained to be 1.2U_{eq}(carrier) for all H atoms.

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
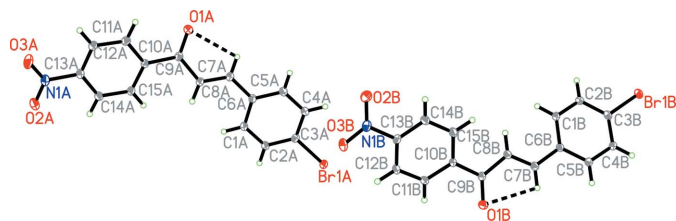

Figure 1
The asymmetric unit of (I), showing 50% probability displacement ellipsoids and the atomic numbering. Dashed lines indicate hydrogen bonds.
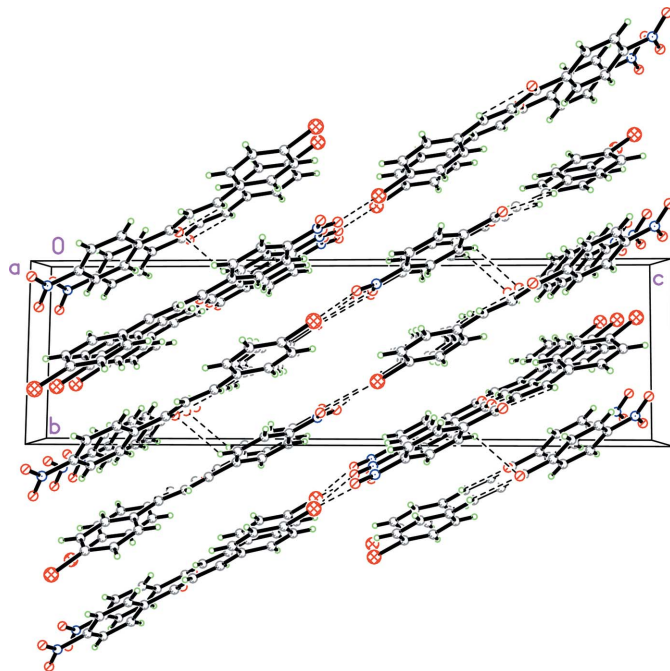

Figure 2
The crystal packing of (I), viewed down the a axis. Hydrogen bonds are shown as dashed lines.

to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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