Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

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

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Key indicators

Single-crystal X-ray study
T = 120 K
Mean σ(C–C) = 0.004 Å
R factor = 0.027
wR factor = 0.058
Data-to-parameter ratio = 15.7

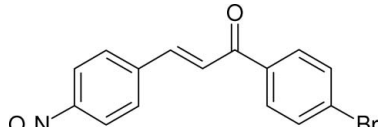
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 18 September 2006
Accepted 28 September 2006

In the approximately planar molecule of the title compound, $C_{15}H_{10}BrNO_3$, the dihedral angle between the two benzene rings is 4.97 (18)°. Intermolecular C—H···O interactions help to form chains of molecules in the crystal structure.

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.



(I)

The geometrical parameters for (I) fall within their expected ranges (Allen *et al.*, 1987). The degree of twisting about the C6—C7 and C9—C10 bonds in (I) (Table 1) is almost the same, but in opposite senses. This results in the C1–C6 and C10–C15 benzene-ring mean planes in (I) being close to parallel [dihedral angle = 4.97 (18)°]. 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)°. The well ordered nitro group in (I) is slightly twisted away from the C10–C15 benzene ring mean plane [dihedral angle = 3.4 (4)°].

A *PLATON* (Spek, 2003) analysis of (I) indicated two possible intermolecular C—H···O interactions (Table 2) that result in chains of molecules (Fig. 2) propagating in either

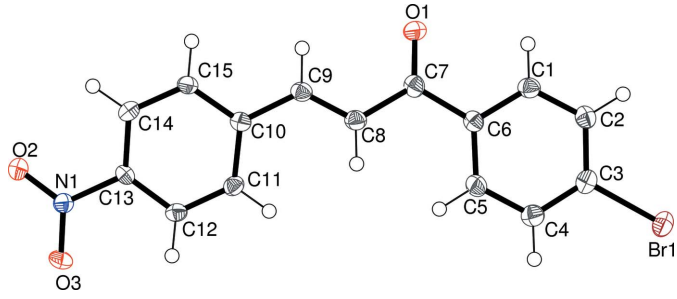


Figure 1
View of the molecular structure of (I) showing 50% probability displacement ellipsoids.

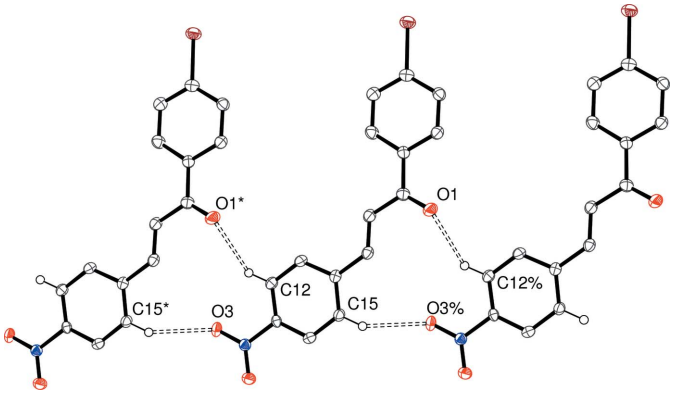


Figure 2
Detail of (I), showing the C—H···O interactions (dashed lines) that link the molecules into [011] and [01$\bar{1}$] chains. Atoms with the suffixes * and % are generated by the symmetry operations (x, $y-1$, $z+1$) and (x, $y+1$, $z-1$), respectively.

[011] or [01$\bar{1}$]. 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

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

Data collection

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

Refinement

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

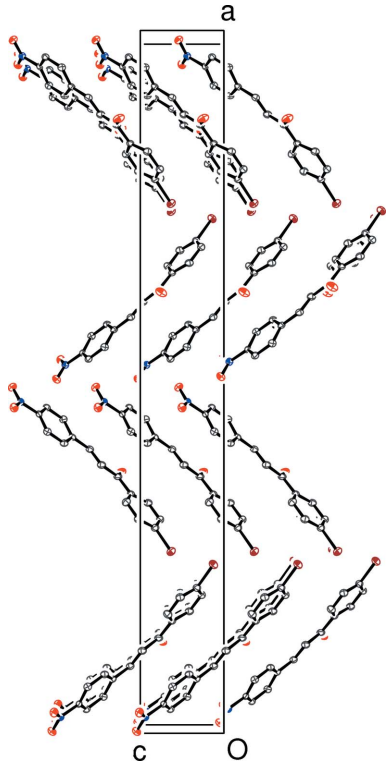


Figure 3
The unit cell contents of (I), viewed down [010]. H atoms have been omitted.

Table 1
Selected torsion angles (°).

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

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···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 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(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.

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supporting information

Acta Cryst. (2006). E**62**, o4829–o4831 [https://doi.org/10.1107/S1600536806039900]

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$V = 1313.92$ (15) Å^3
$Z = 4$
$F(000) = 664$
$D_x = 1.679$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1807 reflections
$\theta = 2.9$–$27.5°$
$\mu = 3.13$ mm^{-1}
$T = 120$ K
Slab, light yellow
0.48 × 0.34 × 0.16 mm

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Nonius KappaCCD diffractometer
Radiation source: fine-focus sealed tube
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Absorption correction: multi-scan (SADABS; Bruker, 2003)
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9881 measured reflections
2833 independent reflections
2452 reflections with $I > 2\sigma(I)$
$R_{int} = 0.034$
$\theta_{max} = 27.6°$, $\theta_{min} = 3.4°$
$h = -55 \rightarrow 51$
$k = -7 \rightarrow 7$
$l = -6 \rightarrow 6$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.027$
$wR(F^2) = 0.058$
$S = 1.03$
2833 reflections
181 parameters
1 restraint
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0103P)^2 + 0.5147P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -0.37$ e Å^{-3}
Absolute structure: Flack (1983), 1143 Friedel pairs
Absolute structure parameter: 0.039 (9)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.32687 (6)	0.5698 (5)	−0.0869 (5)	0.0226 (6)
H1	0.3347	0.7145	−0.1261	0.027*
C2	0.30283 (6)	0.4845 (4)	−0.2341 (5)	0.0231 (6)
H2	0.2941	0.5690	−0.3731	0.028*
C3	0.29161 (6)	0.2713 (5)	−0.1749 (5)	0.0231 (6)
C4	0.30431 (6)	0.1460 (5)	0.0239 (5)	0.0242 (6)
H4	0.2965	0.0007	0.0607	0.029*
C5	0.32863 (6)	0.2330 (4)	0.1705 (6)	0.0241 (7)
H5	0.3376	0.1459	0.3063	0.029*
C6	0.33999 (5)	0.4475 (4)	0.1197 (8)	0.0192 (4)
C7	0.36493 (6)	0.5567 (5)	0.2803 (5)	0.0224 (6)
C8	0.38183 (6)	0.4199 (5)	0.4754 (5)	0.0223 (6)
H8	0.3763	0.2671	0.4973	0.027*
C9	0.40457 (5)	0.5046 (4)	0.6208 (8)	0.0205 (5)
H9	0.4102	0.6560	0.5890	0.025*
C10	0.42189 (6)	0.3854 (4)	0.8269 (5)	0.0180 (5)
C11	0.41295 (6)	0.1732 (4)	0.9179 (5)	0.0207 (6)
H11	0.3953	0.1017	0.8434	0.025*
C12	0.42930 (5)	0.0672 (4)	1.1133 (8)	0.0200 (5)
H12	0.4233	−0.0769	1.1733	0.024*
C13	0.45468 (5)	0.1749 (4)	1.2203 (5)	0.0164 (5)
C14	0.46438 (5)	0.3842 (4)	1.1389 (8)	0.0195 (5)
H14	0.4819	0.4547	1.2162	0.023*
C15	0.44770 (6)	0.4884 (4)	0.9408 (5)	0.0202 (6)
H15	0.4540	0.6323	0.8817	0.024*
N1	0.47161 (5)	0.0649 (4)	1.4359 (4)	0.0193 (5)
O1	0.37058 (4)	0.7549 (3)	0.2512 (4)	0.0333 (5)
O2	0.49310 (4)	0.1664 (3)	1.5394 (4)	0.0244 (4)
O3	0.46321 (4)	−0.1244 (3)	1.5005 (4)	0.0251 (4)
Br1	0.258082 (5)	0.14848 (4)	−0.36943 (8)	0.02868 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0198 (12)	0.0203 (13)	0.0277 (15)	0.0006 (11)	0.0010 (12)	0.0023 (12)
C2	0.0216 (12)	0.0257 (14)	0.0220 (13)	0.0017 (11)	−0.0006 (11)	0.0021 (12)
C3	0.0197 (13)	0.0262 (14)	0.0233 (14)	0.0016 (11)	−0.0001 (11)	−0.0051 (12)
C4	0.0222 (13)	0.0224 (13)	0.0280 (13)	0.0008 (11)	0.0011 (11)	−0.0004 (12)
C5	0.0246 (11)	0.0209 (12)	0.027 (2)	0.0044 (10)	−0.0038 (12)	0.0011 (13)
C6	0.0152 (9)	0.0211 (11)	0.0213 (11)	0.0035 (9)	0.0018 (15)	0.0013 (17)
C7	0.0155 (12)	0.0252 (14)	0.0264 (14)	0.0031 (11)	0.0002 (11)	0.0019 (13)
C8	0.0193 (12)	0.0201 (14)	0.0276 (14)	0.0000 (11)	0.0008 (11)	0.0029 (12)
C9	0.0181 (10)	0.0194 (11)	0.0238 (12)	0.0001 (8)	0.0027 (16)	0.0028 (18)
C10	0.0165 (12)	0.0172 (13)	0.0202 (13)	0.0025 (10)	0.0040 (10)	0.0003 (11)
C11	0.0171 (12)	0.0209 (14)	0.0243 (14)	−0.0027 (10)	0.0002 (11)	−0.0002 (12)

C12	0.0214 (10)	0.0155 (10)	0.0232 (12)	−0.0007 (9)	0.0012 (15)	−0.0009 (16)
C13	0.0171 (11)	0.0178 (13)	0.0143 (11)	0.0032 (10)	0.0026 (9)	0.0019 (10)
C14	0.0180 (9)	0.0199 (12)	0.0206 (11)	−0.0028 (8)	0.0017 (18)	−0.0036 (16)
C15	0.0205 (12)	0.0164 (13)	0.0236 (14)	−0.0009 (10)	−0.0003 (11)	0.0030 (11)
N1	0.0202 (10)	0.0190 (11)	0.0186 (11)	−0.0004 (9)	0.0003 (9)	−0.0001 (10)
O1	0.0304 (10)	0.0221 (10)	0.0473 (12)	−0.0069 (9)	−0.0132 (10)	0.0093 (10)
O2	0.0241 (9)	0.0239 (10)	0.0253 (10)	−0.0015 (8)	−0.0062 (7)	0.0004 (8)
O3	0.0292 (10)	0.0207 (10)	0.0254 (10)	−0.0034 (8)	0.0008 (8)	0.0090 (8)
Br1	0.02627 (12)	0.03238 (14)	0.02741 (13)	−0.00336 (11)	−0.00592 (16)	−0.0030 (2)

Geometric parameters (Å, º)

C1—C2	1.377 (4)	C9—C10	1.474 (4)
C1—C6	1.403 (4)	C9—H9	0.9500
C1—H1	0.9500	C10—C15	1.396 (3)
C2—C3	1.395 (4)	C10—C11	1.404 (3)
C2—H2	0.9500	C11—C12	1.377 (4)
C3—C4	1.375 (4)	C11—H11	0.9500
C3—Br1	1.899 (3)	C12—C13	1.380 (4)
C4—C5	1.388 (4)	C12—H12	0.9500
C4—H4	0.9500	C13—C14	1.382 (3)
C5—C6	1.396 (3)	C13—N1	1.476 (3)
C5—H5	0.9500	C14—C15	1.389 (4)
C6—C7	1.500 (4)	C14—H14	0.9500
C7—O1	1.218 (3)	C15—H15	0.9500
C7—C8	1.481 (4)	N1—O2	1.226 (3)
C8—C9	1.329 (4)	N1—O3	1.232 (3)
C8—H8	0.9500		
C2—C1—C6	121.4 (2)	C8—C9—C10	126.0 (2)
C2—C1—H1	119.3	C8—C9—H9	117.0
C6—C1—H1	119.3	C10—C9—H9	117.0
C1—C2—C3	118.6 (3)	C15—C10—C11	118.5 (2)
C1—C2—H2	120.7	C15—C10—C9	119.2 (2)
C3—C2—H2	120.7	C11—C10—C9	122.3 (2)
C4—C3—C2	121.3 (2)	C12—C11—C10	121.1 (2)
C4—C3—Br1	118.6 (2)	C12—C11—H11	119.5
C2—C3—Br1	120.1 (2)	C10—C11—H11	119.5
C3—C4—C5	119.6 (3)	C11—C12—C13	118.5 (2)
C3—C4—H4	120.2	C11—C12—H12	120.8
C5—C4—H4	120.2	C13—C12—H12	120.8
C4—C5—C6	120.5 (3)	C12—C13—C14	122.8 (3)
C4—C5—H5	119.8	C12—C13—N1	118.6 (2)
C6—C5—H5	119.8	C14—C13—N1	118.6 (2)
C5—C6—C1	118.5 (3)	C13—C14—C15	118.0 (2)
C5—C6—C7	123.2 (3)	C13—C14—H14	121.0
C1—C6—C7	118.3 (2)	C15—C14—H14	121.0
O1—C7—C8	121.4 (2)	C14—C15—C10	121.2 (2)

O1—C7—C6	119.9 (2)	C14—C15—H15	119.4
C8—C7—C6	118.7 (2)	C10—C15—H15	119.4
C9—C8—C7	121.9 (2)	O2—N1—O3	124.0 (2)
C9—C8—H8	119.1	O2—N1—C13	118.3 (2)
C7—C8—H8	119.1	O3—N1—C13	117.7 (2)
C6—C1—C2—C3	−0.3 (4)	C8—C9—C10—C15	172.2 (3)
C1—C2—C3—C4	−0.7 (4)	C8—C9—C10—C11	−9.3 (5)
C1—C2—C3—Br1	179.1 (2)	C15—C10—C11—C12	−0.6 (4)
C2—C3—C4—C5	0.5 (4)	C9—C10—C11—C12	−179.0 (3)
Br1—C3—C4—C5	−179.4 (2)	C10—C11—C12—C13	0.5 (4)
C3—C4—C5—C6	0.8 (4)	C11—C12—C13—C14	−0.2 (4)
C4—C5—C6—C1	−1.8 (4)	C11—C12—C13—N1	178.0 (2)
C4—C5—C6—C7	176.3 (2)	C12—C13—C14—C15	−0.1 (4)
C2—C1—C6—C5	1.5 (4)	N1—C13—C14—C15	−178.2 (2)
C2—C1—C6—C7	−176.7 (2)	C13—C14—C15—C10	0.0 (4)
C5—C6—C7—O1	−169.1 (3)	C11—C10—C15—C14	0.3 (4)
C1—C6—C7—O1	9.1 (4)	C9—C10—C15—C14	178.8 (3)
C5—C6—C7—C8	9.9 (4)	C12—C13—N1—O2	−176.2 (2)
C1—C6—C7—C8	−172.0 (2)	C14—C13—N1—O2	2.0 (3)
O1—C7—C8—C9	−2.4 (4)	C12—C13—N1—O3	3.9 (3)
C6—C7—C8—C9	178.7 (3)	C14—C13—N1—O3	−177.9 (2)
C7—C8—C9—C10	177.4 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
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C15—H15···O3^{ii}	0.95	2.46	3.296 (3)	146

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