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

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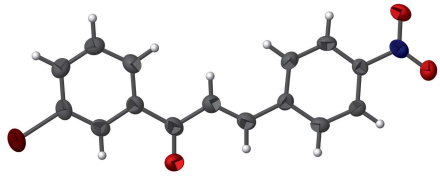
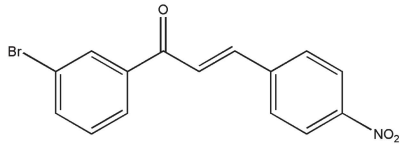
The title compound, $C_{15}H_{10}BrNO_3$, is close to planar, as seen by the dihedral angle of 3.32 (17)° between the bromophenyl and nitrophenyl rings. In the crystal, molecules are linked by weak C—H···O hydrogen bonds, forming chains propagating along the *c*-axis direction.

3D view



Chemical scheme



Structure description

Chalcones have attracted considerable interest because of their major applications in technologies such as optical computing and optical communication systems (Chidan *et al.*, 2015), photonics and optoelectronics. They are also considered to be the precursors of flavonoids and isoflavonoids. Owing to their electronic structure, chalcones also find unique applications as fluorescent probes for sensing metal ions (Kumar *et al.* 2013). In a continuation of our work on the synthesis of new chalcones and studies of their NLO properties (Tejkiran *et al.*, 2016; Chidan *et al.* 2016), we report here the crystal structure of the title compound.

The structure of the molecule is shown in Fig. 1. The molecule is nearly planar, with a dihedral angle of 3.32 (17)° between the bromophenyl and the nitrophenyl rings that are bridged by the enone unit. This value is less than the value of 19.13 (15)° reported earlier between the aromatic rings in the related chalcone derivative (*E*)-3-(2,3-dichlorophenyl)-1-(4-fluorophenyl)prop-2-en-1-one (Naveen *et al.*, 2016). The carbonyl group at C7 lies close to the plane of the olefinic double bond and bromophenyl ring as indicated by the

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

D—H···A	D—H	H···A	D···A	D—H···A
C11—H11A···O3^{i}	0.93	2.54	3.354 (4)	147
C14—H14A···O1^{ii}	0.93	2.52	3.221 (4)	132

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

O1—C7—C8—C9 and O1—C7—C6—C5 torsion angles of −3.9 (6) and 5.2 (5)° respectively.

In the crystal, the molecules are linked *via* weak C—H···O hydrogen bonds (Table 1), forming chains propagating along the *c*-axis direction, Fig. 2.

Synthesis and crystallization

2-Bromoacetophenone (1.99 g, 0.01 mol) was mixed with 4-nitrobenzaldehyde (1.51 g, 0.01 mol) and dissolved in methanol (20 ml). To this, a catalytic amount of NaOH was added slowly, drop-by-drop with constant stirring. The reaction mixture was stirred for 4 h. The resulting crude solid was filtered, washed with distilled water and finally recrystallized from methanol to give the pure chalcone. Single crystals suitable for X-ray diffraction studies were grown by slow evaporation of an acetone solution (m.p. 324–325 K).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

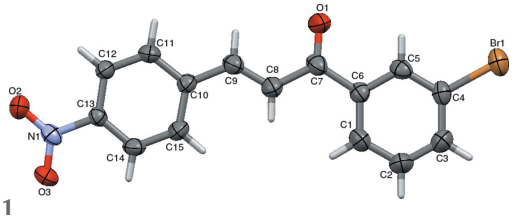


Figure 1
The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.

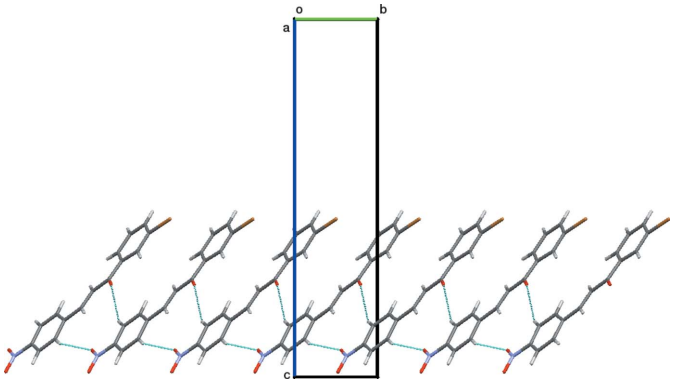


Figure 2
The packing of the molecules, viewed along the *a* axis, with hydrogen bonds drawn as dashed lines.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{15}H_{10}BrNO_3$
M_r	332.14
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	294
a, b, c (Å)	6.0511 (7), 5.0542 (6), 21.841 (3)
β (°)	95.781 (2)
V (Å^3)	664.58 (14)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	3.10
Crystal size (mm)	0.49 × 0.28 × 0.10
Data collection	
Diffractometer	Rigaku Saturn724+
Absorption correction	Multi-scan (*NUMABS*; Rigaku, 1999)
T_{min}, T_{max}	0.312, 0.751
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	8418, 2605, 2325
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.083, 1.06
No. of reflections	2605
No. of parameters	181
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, −0.40
Absolute structure	Flack (1983)
Absolute structure parameter	0.028 (11)

Computer programs: *CrystalClear SM-Expert* (Rigaku, 2011), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x170287 [https://doi.org/10.1107/S2414314617002875]

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Crystal data

$C_{15}H_{10}BrNO_3$
M_r = 332.14
Monoclinic, $P2_1$
Hall symbol: P 2yb
a = 6.0511 (7) Å
b = 5.0542 (6) Å
c = 21.841 (3) Å
β = 95.781 (2)°
V = 664.58 (14) Å^3
Z = 2
$F(000)$ = 332
D_x = 1.660 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2325 reflections
θ = 1.9–26.1°
μ = 3.10 mm^{-1}
T = 294 K
Rectangle, brown
0.49 × 0.28 × 0.10 mm

Data collection

Rigaku Saturn724+ diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 18.4 pixels mm^{-1}
profile data from ω–scans
Absorption correction: multi-scan (NUMABS; Rigaku, 1999)
T_{min} = 0.312, T_{max} = 0.751
8418 measured reflections
2605 independent reflections
2325 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 26.1°, θ_{min} = 1.9°
h = −7→7
k = −6→6
l = −27→24

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.083
S = 1.06
2605 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
$w = 1/[\sigma^2(F_o^2) + (0.0421P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}
Absolute structure: Flack (1983)
Absolute structure parameter: 0.028 (11)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating -R-factor-obs etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Br1	0.10940 (5)	1.49979 (11)	0.55889 (2)	0.0536 (1)
O1	0.1299 (4)	0.7918 (8)	0.74119 (13)	0.0805 (13)
O2	0.8278 (4)	−0.4766 (7)	0.98538 (11)	0.0523 (8)
O3	1.0879 (4)	−0.4357 (5)	0.92554 (12)	0.0544 (10)
N1	0.9084 (4)	−0.3727 (6)	0.94205 (13)	0.0397 (9)
C1	0.5966 (6)	0.8764 (8)	0.65218 (17)	0.0499 (11)
C2	0.6499 (5)	1.0205 (12)	0.60163 (17)	0.0576 (13)
C3	0.5076 (6)	1.1998 (8)	0.57345 (18)	0.0522 (12)
C4	0.3066 (5)	1.2470 (7)	0.59803 (15)	0.0405 (11)
C5	0.2521 (6)	1.1097 (7)	0.64856 (17)	0.0401 (11)
C6	0.3956 (5)	0.9202 (6)	0.67594 (16)	0.0384 (11)
C7	0.3196 (6)	0.7626 (8)	0.72774 (16)	0.0461 (12)
C8	0.4693 (6)	0.5698 (7)	0.76037 (16)	0.0470 (14)
C9	0.4138 (6)	0.4312 (7)	0.80724 (17)	0.0435 (13)
C10	0.5470 (5)	0.2282 (7)	0.84194 (15)	0.0359 (10)
C11	0.4689 (5)	0.1157 (7)	0.89396 (16)	0.0409 (10)
C12	0.5857 (5)	−0.0774 (6)	0.92742 (17)	0.0375 (11)
C13	0.7850 (5)	−0.1623 (6)	0.90817 (15)	0.0326 (10)
C14	0.8681 (5)	−0.0549 (7)	0.85751 (16)	0.0421 (13)
C15	0.7494 (6)	0.1405 (7)	0.82458 (16)	0.0434 (11)
H1A	0.69530	0.75090	0.67010	0.0600*
H2A	0.78680	0.99340	0.58670	0.0690*
H3A	0.54270	1.28940	0.53850	0.0630*
H5A	0.11820	1.14370	0.66450	0.0480*
H8A	0.60940	0.54470	0.74730	0.0560*
H9A	0.27440	0.46550	0.81990	0.0530*
H11A	0.33430	0.17310	0.90630	0.0490*
H12A	0.53230	−0.14960	0.96220	0.0450*
H14A	1.00300	−0.11330	0.84550	0.0510*
H15A	0.80550	0.21450	0.79040	0.0520*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0622 (2)	0.0424 (2)	0.0541 (2)	0.0079 (2)	−0.0041 (2)	0.0068 (2)
O1	0.0605 (17)	0.120 (3)	0.066 (2)	0.0404 (18)	0.0305 (15)	0.0444 (19)

O2	0.0533 (12)	0.0489 (16)	0.0559 (14)	0.0060 (14)	0.0111 (10)	0.0179 (16)
O3	0.0488 (13)	0.052 (2)	0.0643 (17)	0.0202 (11)	0.0158 (12)	0.0045 (12)
N1	0.0420 (16)	0.0328 (15)	0.0434 (18)	0.0072 (11)	−0.0004 (13)	−0.0078 (12)
C1	0.0431 (18)	0.054 (2)	0.052 (2)	0.0101 (16)	0.0022 (17)	0.0085 (17)
C2	0.0443 (17)	0.065 (3)	0.066 (2)	0.006 (2)	0.0182 (15)	0.016 (3)
C3	0.051 (2)	0.054 (2)	0.053 (2)	−0.0019 (19)	0.0127 (17)	0.0123 (19)
C4	0.0490 (19)	0.0328 (18)	0.0381 (19)	0.0016 (14)	−0.0038 (15)	0.0002 (14)
C5	0.0385 (17)	0.0447 (19)	0.037 (2)	0.0058 (14)	0.0032 (15)	−0.0062 (14)
C6	0.0427 (18)	0.040 (2)	0.0321 (18)	0.0037 (13)	0.0024 (14)	−0.0023 (12)
C7	0.049 (2)	0.052 (2)	0.037 (2)	0.0157 (17)	0.0036 (16)	−0.0008 (16)
C8	0.0482 (19)	0.053 (3)	0.041 (2)	0.0103 (16)	0.0100 (16)	0.0053 (15)
C9	0.0398 (16)	0.049 (3)	0.042 (2)	0.0085 (14)	0.0052 (15)	−0.0002 (14)
C10	0.0390 (16)	0.0366 (18)	0.0328 (18)	0.0010 (14)	0.0065 (13)	0.0016 (13)
C11	0.0342 (16)	0.0449 (18)	0.045 (2)	0.0069 (14)	0.0108 (15)	0.0003 (15)
C12	0.0398 (16)	0.034 (2)	0.0403 (19)	0.0021 (12)	0.0120 (14)	0.0030 (12)
C13	0.0336 (15)	0.0270 (17)	0.0370 (18)	0.0019 (12)	0.0027 (13)	0.0000 (13)
C14	0.0339 (15)	0.050 (3)	0.044 (2)	0.0070 (14)	0.0117 (14)	−0.0025 (15)
C15	0.0463 (19)	0.047 (2)	0.039 (2)	0.0014 (15)	0.0140 (16)	0.0061 (16)

Geometric parameters (Å, º)

Br1—C4	1.893 (3)	C10—C15	1.391 (5)
O1—C7	1.222 (4)	C11—C12	1.372 (5)
O2—N1	1.226 (4)	C12—C13	1.385 (4)
O3—N1	1.221 (4)	C13—C14	1.373 (5)
N1—C13	1.458 (4)	C14—C15	1.380 (5)
C1—C2	1.388 (6)	C1—H1A	0.9300
C1—C6	1.387 (5)	C2—H2A	0.9300
C2—C3	1.355 (6)	C3—H3A	0.9300
C3—C4	1.399 (5)	C5—H5A	0.9300
C4—C5	1.372 (5)	C8—H8A	0.9300
C5—C6	1.387 (5)	C9—H9A	0.9300
C6—C7	1.494 (5)	C11—H11A	0.9300
C7—C8	1.466 (5)	C12—H12A	0.9300
C8—C9	1.312 (5)	C14—H14A	0.9300
C9—C10	1.468 (5)	C15—H15A	0.9300
C10—C11	1.395 (5)		

O2—N1—O3	123.5 (3)	N1—C13—C14	119.2 (3)
O2—N1—C13	118.8 (3)	C12—C13—C14	121.6 (3)
O3—N1—C13	117.8 (3)	C13—C14—C15	119.3 (3)
C2—C1—C6	119.8 (3)	C10—C15—C14	120.8 (3)
C1—C2—C3	121.7 (3)	C2—C1—H1A	120.00
C2—C3—C4	118.5 (3)	C6—C1—H1A	120.00
Br1—C4—C3	118.4 (3)	C1—C2—H2A	119.00
Br1—C4—C5	120.9 (2)	C3—C2—H2A	119.00
C3—C4—C5	120.8 (3)	C2—C3—H3A	121.00
C4—C5—C6	120.4 (3)	C4—C3—H3A	121.00

C1—C6—C5	118.9 (3)	C4—C5—H5A	120.00
C1—C6—C7	123.1 (3)	C6—C5—H5A	120.00
C5—C6—C7	117.9 (3)	C7—C8—H8A	119.00
O1—C7—C6	119.1 (3)	C9—C8—H8A	119.00
O1—C7—C8	120.9 (4)	C8—C9—H9A	116.00
C6—C7—C8	120.0 (3)	C10—C9—H9A	116.00
C7—C8—C9	122.7 (3)	C10—C11—H11A	119.00
C8—C9—C10	127.3 (3)	C12—C11—H11A	119.00
C9—C10—C11	119.5 (3)	C11—C12—H12A	121.00
C9—C10—C15	122.4 (3)	C13—C12—H12A	121.00
C11—C10—C15	118.2 (3)	C13—C14—H14A	120.00
C10—C11—C12	121.7 (3)	C15—C14—H14A	120.00
C11—C12—C13	118.5 (3)	C10—C15—H15A	120.00
N1—C13—C12	119.3 (3)	C14—C15—H15A	120.00
O2—N1—C13—C12	2.9 (5)	C5—C6—C7—C8	−176.8 (3)
O2—N1—C13—C14	−176.4 (3)	O1—C7—C8—C9	−3.9 (6)
O3—N1—C13—C12	−177.0 (3)	C6—C7—C8—C9	178.1 (3)
O3—N1—C13—C14	3.7 (4)	C7—C8—C9—C10	178.0 (3)
C6—C1—C2—C3	−1.8 (7)	C8—C9—C10—C11	174.7 (4)
C2—C1—C6—C5	−0.4 (6)	C8—C9—C10—C15	−5.9 (6)
C2—C1—C6—C7	176.2 (4)	C9—C10—C11—C12	179.1 (3)
C1—C2—C3—C4	2.8 (7)	C15—C10—C11—C12	−0.4 (5)
C2—C3—C4—Br1	179.5 (3)	C9—C10—C15—C14	−178.6 (3)
C2—C3—C4—C5	−1.7 (6)	C11—C10—C15—C14	0.8 (5)
Br1—C4—C5—C6	178.4 (3)	C10—C11—C12—C13	−0.6 (5)
C3—C4—C5—C6	−0.4 (5)	C11—C12—C13—N1	−178.2 (3)
C4—C5—C6—C1	1.4 (5)	C11—C12—C13—C14	1.1 (5)
C4—C5—C6—C7	−175.4 (3)	N1—C13—C14—C15	178.7 (3)
C1—C6—C7—O1	−171.4 (4)	C12—C13—C14—C15	−0.6 (5)
C1—C6—C7—C8	6.6 (5)	C13—C14—C15—C10	−0.3 (5)
C5—C6—C7—O1	5.2 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11*A*···O3^{i}	0.93	2.54	3.354 (4)	147
C14—H14*A*···O1^{ii}	0.93	2.52	3.221 (4)	132

Symmetry codes: (i) *x*−1, *y*+1, *z*; (ii) *x*+1, *y*−1, *z*.