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

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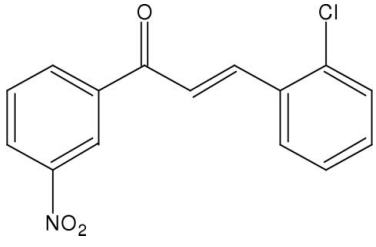
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.003 Å; R factor = 0.041; wR factor = 0.112; data-to-parameter ratio = 13.4.

Geometric parameters of the title compound, $C_{15}H_{10}ClNO_3$, a chalcone derivative, are in the usual ranges. The molecules are almost planar and crystallize in stacks with an interplanar distance of approximately 3.4 Å. No classical hydrogen bonds were found.

Related literature

For related structures, see: Yathirajan, Mayekar, Narayana *et al.* (2007); Fischer *et al.* (2007); Yathirajan, Mayekar, Sarojini *et al.* (2007). For related literature, see: Di Carlo *et al.* (1999); Dimmock *et al.* (1999); Go *et al.* (2005); Fichou *et al.* (1988); Goto *et al.* (1991); Uchida *et al.* (1998); Sarojini *et al.* (2006).



Experimental

Crystal data

$C_{15}H_{10}ClNO_3$
M_r = 287.69
Monoclinic, $P2_1/n$
a = 7.3643 (10) Å
b = 12.8295 (11) Å
c = 13.9452 (14) Å
β = 93.898 (9)°
V = 1314.5 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.30 mm^{-1}
T = 173 (2) K
0.43 × 0.40 × 0.37 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.883, T_{max} = 0.898
7978 measured reflections
2433 independent reflections
1977 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.112
S = 1.04
2433 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2310).

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supplementary materials

Acta Cryst. (2007). E**63**, o3211 [**doi:10.1107/S1600536807026815**]

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

B. K. Sarojini, H. S. Yathirajan, K. Lakshmana, B. Narayana and M. Bolte

Comment

Chalcones are one of the major classes of natural products with widespread distribution in fruits, vegetables, spices, tea and soy based foodstuff have been recently subjects of great interest for their interesting pharmacological activities. Reviews on the bioactivities of varieties of chalcones are published in the literature recently. Recently, it has been noted that, among many organic compounds reported for their second harmonic generation, chalcone derivatives are known for their excellent blue light transmittance and good crystallizability. In continuation of our broad programme on chalcones, the present paper reports the crystal structure of a newly synthesized chalcone.

Geometric parameters of the title compound are in the usual ranges. The molecules are almost planar (r.m.s. deviation for all non-H atoms 0.113 Å) and crystallize in stacks. There is no classical hydrogen bonds.

Experimental

To a thoroughly stirred solution of 1-(3-nitrophenyl)ethanone (1.65 g, 0.01 mol) and 2-chlorobenzaldehyde (1.40 g, 0.01 mol) in 25 ml me thanol, 5 ml of 30% KOH solution was added. The solution was stirred overnight and filtered. The product was crystallized from acetone by slow evaporation (m.p.: 410–412 K). Analysis for $C_{15}H_{10}ClNO_3$: Found (Calculated): C 62.56 (62.62), H 3.41 (3.50), N 4.81 (4.87).

Refinement

H atoms were found in a difference map, but they were refined using a riding model with C—H = 0.95Å and U_{iso}(H) = 1.2U_{eq}(C).

Figures

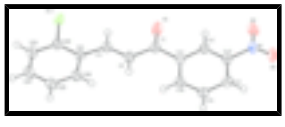


Fig. 1. Perspective view of the title compound with the atom numbering. Displacement ellipsoids are at the 50% probability level.

(2E)-3-(2-Chlorophenyl)-1-(3-nitrophenyl)prop-2-en-1-one

Crystal data

$C_{15}H_{10}ClNO_3$	F_{000} = 592
M_r = 287.69	D_x = 1.454 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å

Hall symbol: -P 2yn	Cell parameters from 7582 reflections
a = 7.3643 (10) Å	θ = 3.5–25.7º
b = 12.8295 (11) Å	μ = 0.30 mm^{-1}
c = 13.9452 (14) Å	T = 173 (2) K
β = 93.898 (9)º	Block, brown
V = 1314.5 (2) $Å^3$	0.43 × 0.40 × 0.37 mm
Z = 4	

Data collection

STOE IPDS II two-circle diffractometer	2433 independent reflections
Radiation source: fine-focus sealed tube	1977 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.055
T = 173(2) K	θ_{max} = 25.6º
ω scans	θ_{min} = 3.5º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	$h = -7 \rightarrow 8$
T_{min} = 0.883, T_{max} = 0.898	$k = -13 \rightarrow 15$
7978 measured reflections	$l = -16 \rightarrow 16$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.041	$w = 1/[\sigma^2(F_o^2) + (0.0678P)^2 + 0.1649P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.112	$(\Delta/\sigma)_{max}$ = 0.001
S = 1.04	$\Delta\rho_{max}$ = 0.26 e $Å^{-3}$
2433 reflections	$\Delta\rho_{min}$ = −0.28 e $Å^{-3}$
182 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.009 (2)
Secondary atom site location: difference Fourier map	

Special details

Experimental. ;

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.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness 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 threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculat-

ing *R*-factors(gt) *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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.20045 (8)	0.15573 (4)	0.60287 (3)	0.03658 (19)
N1	0.5177 (2)	0.91050 (12)	0.71148 (11)	0.0321 (4)
O1	0.3613 (3)	0.52709 (11)	0.68321 (10)	0.0594 (6)
O2	0.5581 (2)	1.00014 (10)	0.68882 (11)	0.0470 (4)
O3	0.5469 (2)	0.87440 (12)	0.79277 (9)	0.0418 (4)
C1	0.3232 (3)	0.55836 (14)	0.60200 (13)	0.0303 (5)
C2	0.2583 (3)	0.48688 (15)	0.52359 (13)	0.0314 (5)
H2	0.2269	0.5149	0.4616	0.038*
C3	0.2423 (3)	0.38477 (14)	0.53709 (12)	0.0275 (4)
H3	0.2738	0.3591	0.5999	0.033*
C11	0.3414 (3)	0.67301 (13)	0.58022 (12)	0.0245 (4)
C12	0.4164 (3)	0.73743 (14)	0.65350 (12)	0.0253 (4)
H12	0.4546	0.7093	0.7146	0.030*
C13	0.4339 (3)	0.84219 (13)	0.63547 (12)	0.0247 (4)
C14	0.3776 (3)	0.88744 (15)	0.54758 (13)	0.0288 (4)
H14	0.3895	0.9603	0.5377	0.035*
C15	0.3042 (3)	0.82363 (15)	0.47535 (13)	0.0299 (4)
H15	0.2652	0.8526	0.4147	0.036*
C16	0.2868 (3)	0.71654 (14)	0.49089 (12)	0.0276 (4)
H16	0.2377	0.6730	0.4404	0.033*
C21	0.1804 (3)	0.30800 (14)	0.46390 (12)	0.0244 (4)
C22	0.1591 (3)	0.20200 (14)	0.48547 (12)	0.0261 (4)
C23	0.0989 (3)	0.12985 (15)	0.41637 (14)	0.0326 (5)
H23	0.0856	0.0587	0.4333	0.039*
C24	0.0579 (3)	0.16236 (16)	0.32188 (14)	0.0356 (5)
H24	0.0165	0.1134	0.2741	0.043*
C25	0.0778 (3)	0.26644 (16)	0.29803 (14)	0.0349 (5)
H25	0.0495	0.2890	0.2339	0.042*
C26	0.1392 (3)	0.33786 (14)	0.36791 (13)	0.0305 (4)
H26	0.1537	0.4088	0.3503	0.037*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0563 (4)	0.0228 (3)	0.0303 (3)	0.0022 (2)	0.0010 (2)	0.00355 (17)
N1	0.0376 (11)	0.0251 (8)	0.0332 (9)	−0.0014 (8)	−0.0014 (7)	−0.0066 (7)
O1	0.1133 (16)	0.0240 (8)	0.0363 (8)	−0.0050 (9)	−0.0284 (9)	0.0049 (6)
O2	0.0688 (12)	0.0213 (8)	0.0491 (9)	−0.0094 (8)	−0.0087 (8)	−0.0055 (6)
O3	0.0591 (11)	0.0380 (8)	0.0269 (7)	−0.0061 (8)	−0.0064 (6)	−0.0040 (6)
C1	0.0378 (12)	0.0213 (9)	0.0306 (10)	−0.0005 (8)	−0.0053 (8)	0.0002 (7)
C2	0.0416 (13)	0.0222 (9)	0.0297 (10)	−0.0025 (9)	−0.0034 (8)	0.0006 (7)
C3	0.0321 (11)	0.0231 (9)	0.0266 (9)	0.0005 (8)	−0.0026 (7)	0.0004 (7)

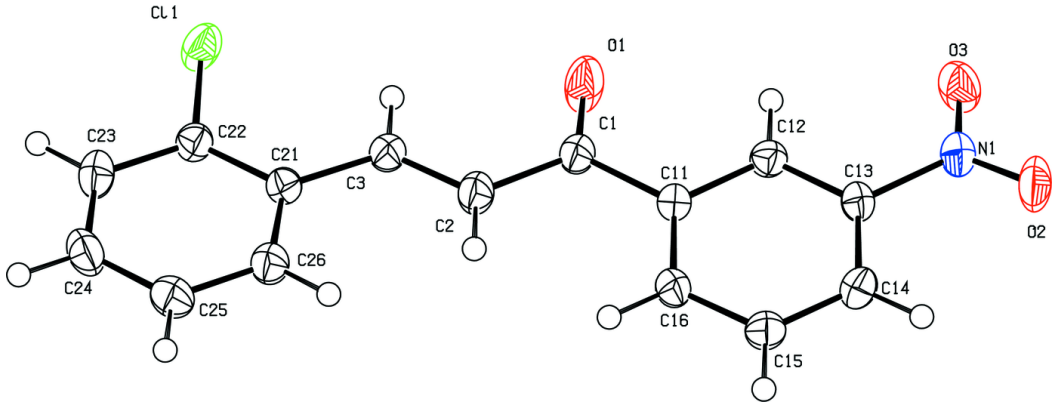
C11	0.0257 (10)	0.0211 (9)	0.0263 (9)	−0.0003 (8)	−0.0003 (7)	−0.0018 (7)
C12	0.0279 (10)	0.0243 (9)	0.0236 (9)	0.0016 (8)	0.0002 (7)	−0.0001 (7)
C13	0.0269 (10)	0.0226 (9)	0.0245 (9)	−0.0018 (8)	0.0018 (7)	−0.0043 (7)
C14	0.0331 (11)	0.0217 (9)	0.0317 (9)	−0.0003 (8)	0.0033 (8)	0.0018 (7)
C15	0.0359 (11)	0.0275 (10)	0.0257 (9)	0.0011 (8)	−0.0032 (8)	0.0030 (7)
C16	0.0320 (11)	0.0249 (10)	0.0251 (9)	−0.0008 (8)	−0.0029 (8)	−0.0032 (7)
C21	0.0230 (10)	0.0229 (9)	0.0270 (9)	−0.0008 (7)	0.0006 (7)	−0.0007 (7)
C22	0.0268 (10)	0.0240 (9)	0.0274 (9)	0.0008 (8)	0.0021 (7)	−0.0011 (7)
C23	0.0356 (12)	0.0235 (9)	0.0392 (11)	−0.0049 (9)	0.0058 (8)	−0.0041 (8)
C24	0.0348 (12)	0.0356 (11)	0.0359 (11)	−0.0054 (9)	−0.0023 (8)	−0.0119 (8)
C25	0.0397 (12)	0.0368 (11)	0.0273 (9)	−0.0003 (10)	−0.0048 (8)	−0.0008 (8)
C26	0.0348 (11)	0.0256 (9)	0.0306 (10)	−0.0019 (9)	−0.0012 (8)	0.0004 (7)

Geometric parameters (Å, °)

Cl1—C22	1.7486 (18)	C14—C15	1.380 (3)
N1—O3	1.230 (2)	C14—H14	0.9500
N1—O2	1.234 (2)	C15—C16	1.398 (3)
N1—C13	1.478 (2)	C15—H15	0.9500
O1—C1	1.216 (2)	C16—H16	0.9500
C1—C2	1.481 (2)	C21—C22	1.404 (3)
C1—C11	1.510 (2)	C21—C26	1.406 (2)
C2—C3	1.330 (3)	C22—C23	1.387 (3)
C2—H2	0.9500	C23—C24	1.395 (3)
C3—C21	1.468 (2)	C23—H23	0.9500
C3—H3	0.9500	C24—C25	1.386 (3)
C11—C12	1.399 (2)	C24—H24	0.9500
C11—C16	1.399 (2)	C25—C26	1.391 (3)
C12—C13	1.375 (3)	C25—H25	0.9500
C12—H12	0.9500	C26—H26	0.9500
C13—C14	1.394 (2)		
O3—N1—O2	123.84 (16)	C14—C15—C16	120.36 (16)
O3—N1—C13	118.42 (15)	C14—C15—H15	119.8
O2—N1—C13	117.71 (15)	C16—C15—H15	119.8
O1—C1—C2	121.70 (17)	C15—C16—C11	120.44 (16)
O1—C1—C11	119.39 (16)	C15—C16—H16	119.8
C2—C1—C11	118.90 (15)	C11—C16—H16	119.8
C3—C2—C1	122.19 (17)	C22—C21—C26	116.61 (16)
C3—C2—H2	118.9	C22—C21—C3	122.33 (16)
C1—C2—H2	118.9	C26—C21—C3	121.06 (17)
C2—C3—C21	126.06 (17)	C23—C22—C21	122.20 (17)
C2—C3—H3	117.0	C23—C22—Cl1	116.80 (14)
C21—C3—H3	117.0	C21—C22—Cl1	120.96 (13)
C12—C11—C16	119.34 (16)	C22—C23—C24	119.66 (18)
C12—C11—C1	117.70 (15)	C22—C23—H23	120.2
C16—C11—C1	122.96 (15)	C24—C23—H23	120.2
C13—C12—C11	118.77 (16)	C25—C24—C23	119.66 (17)
C13—C12—H12	120.6	C25—C24—H24	120.2
C11—C12—H12	120.6	C23—C24—H24	120.2

C12—C13—C14	122.83 (16)	C24—C25—C26	120.08 (18)
C12—C13—N1	119.22 (16)	C24—C25—H25	120.0
C14—C13—N1	117.94 (15)	C26—C25—H25	120.0
C15—C14—C13	118.25 (17)	C25—C26—C21	121.78 (18)
C15—C14—H14	120.9	C25—C26—H26	119.1
C13—C14—H14	120.9	C21—C26—H26	119.1
O1—C1—C2—C3	−1.7 (3)	C13—C14—C15—C16	0.2 (3)
C11—C1—C2—C3	178.7 (2)	C14—C15—C16—C11	0.9 (3)
C1—C2—C3—C21	−179.60 (19)	C12—C11—C16—C15	−1.1 (3)
O1—C1—C11—C12	5.3 (3)	C1—C11—C16—C15	178.94 (19)
C2—C1—C11—C12	−175.09 (18)	C2—C3—C21—C22	−176.8 (2)
O1—C1—C11—C16	−174.8 (2)	C2—C3—C21—C26	3.1 (3)
C2—C1—C11—C16	4.9 (3)	C26—C21—C22—C23	−0.6 (3)
C16—C11—C12—C13	0.2 (3)	C3—C21—C22—C23	179.33 (18)
C1—C11—C12—C13	−179.82 (18)	C26—C21—C22—Cl1	−178.37 (14)
C11—C12—C13—C14	0.9 (3)	C3—C21—C22—Cl1	1.6 (3)
C11—C12—C13—N1	−178.30 (17)	C21—C22—C23—C24	0.1 (3)
O3—N1—C13—C12	−9.7 (3)	Cl1—C22—C23—C24	178.00 (16)
O2—N1—C13—C12	168.70 (19)	C22—C23—C24—C25	0.0 (3)
O3—N1—C13—C14	171.00 (18)	C23—C24—C25—C26	0.3 (3)
O2—N1—C13—C14	−10.5 (3)	C24—C25—C26—C21	−0.8 (3)
C12—C13—C14—C15	−1.1 (3)	C22—C21—C26—C25	0.9 (3)
N1—C13—C14—C15	178.10 (17)	C3—C21—C26—C25	−179.01 (19)

Fig. 1


Cl1
O1
O3
C23
C22
C21
C3
C1
C12
N1
C2
C11
C13
O2
C26
C24
C25
C14
C16
C15