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(*E*)-1-(4-Nitrophenyl)-3-phenylprop-2-en-1-one

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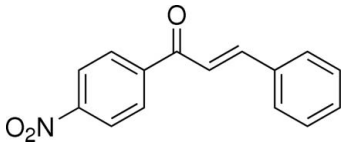
Key indicators: single-crystal X-ray study; T = 93 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.097; data-to-parameter ratio = 15.6.

In the title compound, $C_{15}H_{11}NO_3$, the configuration of the keto group with respect to the olefinic double bond is *s–cis*. The two benzene rings form a dihedral angle of 5.00 (5)°. The molecules are linked into a two-dimensional network parallel to ($\bar{1}$04) by C—H···O hydrogen bonds.

Related literature

For the biological activity of chalcone derivatives, see: Dimmock *et al.* (1999). For the synthesis, see: Cocconcelli *et al.* (2008).



Experimental

Crystal data

$C_{15}H_{11}NO_3$
M_r = 253.25
Monoclinic, $P2_1/c$
a = 6.2139 (10) Å
b = 13.159 (2) Å
c = 14.450 (3) Å
β = 92.106 (3)°
V = 1180.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 93 K
0.50 × 0.18 × 0.18 mm

Data collection

Rigaku SPIDER diffractometer
Absorption correction: none
9403 measured reflections
2687 independent reflections
2264 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.097
S = 1.00
2687 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C1—H1···O1^{i}	0.95	2.47	3.3314 (15)	150
C5—H5···O3^{ii}	0.95	2.56	3.4635 (16)	160

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+2, y+\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *RAPID-AUTO* (Rigaku, 2004); cell refinement: *RAPID-AUTO*; data reduction: *RAPID-AUTO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

The authors thank the Centre for Testing and Analysis, Cheng Du Branch, Chinese Academy of Sciences, for analytical support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2913).

References

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Dimmock, J. R., Elias, D. W., Beazely, M. A. & Kandepu, N. M. (1999). *Curr. Med. Chem.* **6**, 1125–1149.
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supporting information

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S1. Comment

Chalcone derivatives are a class of important compounds that possess antiprotzoal, antihelmintic, amoebicidal, anti-ulcer, antiviral, insecticidal, antibacterial, anticancer, cytotoxic and immunosuppressive activities (Dimmock *et al.*, 1999). The crystal structures of some chalcone derivatives have been reported. We report here the crystal structure of the title compound.

Bond lengths and angles in the title molecule are normal. The configuration of the keto group with respect to the olefinic double bond is typically *s-cis*, with a O1—C9—C8—C7 torsion angle of 0.5 (2)° (Fig. 1). The N1/O2/O3 and C10-C15 planes form a dihedral angle of 10.80 (11)°. The two benzene rings (C10-C15 and C1-C6) form a dihedral angle of 5.00 (5)°. The crystal packing is stabilized by C—H···O hydrogen bonds (Table 1). The molecules are linked into a two-dimensional network parallel to the ($\bar{1}$ 0 4) by the above hydrogen bonds.

S2. Experimental

The title compound was synthesized according to the method reported in the literature (Cocconcelli *et al.*, 2008). Yellow single crystals suitable for X-ray diffraction were obtained by slow evaporation of a acetone solution.

S3. Refinement

All H atoms were placed in calculated positions, with C-H = 0.95 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C).

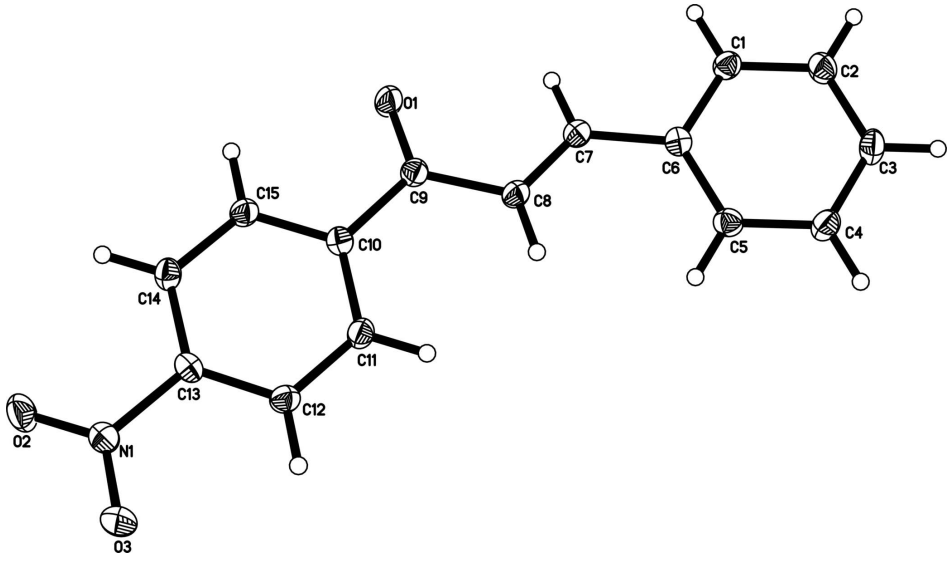

Figure 1

The molecular structure of the title compound, showing 50% probability displacement ellipsoids and the atomic numbering.

(*E*)-1-(4-Nitrophenyl)-3-phenylprop-2-en-1-one

Crystal data

$C_{15}H_{11}NO_3$
$M_r = 253.25$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 6.2139\ (10)$ Å
$b = 13.159\ (2)$ Å
$c = 14.450\ (3)$ Å
$\beta = 92.106\ (3)°$
$V = 1180.8\ (3)$ Å^3
$Z = 4$
$F(000) = 528$
$D_x = 1.425$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3448 reflections
$\theta = 3.1–27.5°$
$\mu = 0.10$ mm^{-1}
$T = 93$ K
Needle, yellow
0.50 × 0.18 × 0.18 mm

Data collection

Rigaku SPIDER diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
9403 measured reflections
2687 independent reflections
2264 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$
$h = -8\rightarrow7$
$k = -17\rightarrow17$
$l = -18\rightarrow15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.097$
$S = 1.00$
2687 reflections
172 parameters
0 restraints
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

$w = 1/[\sigma^2(F_o^2) + (0.0516P)^2 + 0.336P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.36$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ e Å^{-3}

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.

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 $F^2 > \sigma(F^2)$ is used only for calculating *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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.19885 (14)	0.39882 (7)	0.06264 (7)	0.0243 (2)
O2	0.89968 (15)	0.02961 (7)	0.20944 (7)	0.0266 (2)
O3	1.11753 (14)	0.14090 (7)	0.27163 (7)	0.0272 (2)
N1	0.94974 (16)	0.11770 (8)	0.22851 (7)	0.0185 (2)
C1	0.11212 (19)	0.77346 (9)	0.04561 (8)	0.0179 (3)
H1	−0.0164	0.7395	0.0258	0.021*
C2	0.1184 (2)	0.87899 (9)	0.04625 (9)	0.0209 (3)
H2	−0.0059	0.9169	0.0277	0.025*
C3	0.3061 (2)	0.92892 (9)	0.07402 (9)	0.0221 (3)
H3	0.3104	1.0011	0.0741	0.027*
C4	0.4885 (2)	0.87379 (9)	0.10183 (8)	0.0205 (3)
H4	0.6170	0.9083	0.1206	0.025*
C5	0.48224 (19)	0.76832 (9)	0.10203 (8)	0.0180 (3)
H5	0.6066	0.7309	0.1214	0.022*
C6	0.29377 (19)	0.71675 (9)	0.07389 (8)	0.0158 (3)
C7	0.27514 (19)	0.60597 (9)	0.07315 (8)	0.0163 (2)
H7	0.1469	0.5789	0.0451	0.020*
C8	0.41785 (19)	0.53830 (9)	0.10745 (8)	0.0169 (3)
H8	0.5496	0.5604	0.1362	0.020*
C9	0.36764 (19)	0.42863 (9)	0.10009 (8)	0.0167 (3)
C10	0.52508 (19)	0.35096 (9)	0.13838 (8)	0.0155 (2)
C11	0.72971 (19)	0.37564 (9)	0.17453 (8)	0.0173 (3)
H11	0.7733	0.4448	0.1780	0.021*
C12	0.87037 (19)	0.29959 (9)	0.20556 (8)	0.0172 (3)
H12	1.0095	0.3158	0.2308	0.021*
C13	0.80212 (19)	0.19972 (9)	0.19868 (8)	0.0158 (3)
C14	0.59903 (19)	0.17265 (9)	0.16446 (8)	0.0174 (3)
H14	0.5558	0.1034	0.1618	0.021*
C15	0.46102 (19)	0.24900 (9)	0.13438 (8)	0.0172 (3)
H15	0.3209	0.2322	0.1107	0.021*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0198 (5)	0.0168 (4)	0.0355 (5)	−0.0023 (4)	−0.0093 (4)	0.0018 (4)
O2	0.0289 (5)	0.0153 (4)	0.0349 (5)	0.0044 (4)	−0.0061 (4)	−0.0033 (4)
O3	0.0188 (5)	0.0252 (5)	0.0367 (6)	0.0010 (4)	−0.0095 (4)	0.0031 (4)
N1	0.0180 (5)	0.0183 (5)	0.0190 (5)	0.0018 (4)	0.0005 (4)	0.0008 (4)
C1	0.0174 (6)	0.0176 (6)	0.0184 (6)	−0.0015 (5)	−0.0016 (5)	0.0006 (5)
C2	0.0212 (6)	0.0174 (6)	0.0238 (6)	0.0029 (5)	−0.0032 (5)	0.0021 (5)
C3	0.0278 (7)	0.0132 (5)	0.0250 (6)	−0.0008 (5)	−0.0022 (5)	−0.0002 (5)
C4	0.0206 (6)	0.0186 (6)	0.0221 (6)	−0.0039 (5)	−0.0017 (5)	−0.0014 (5)
C5	0.0168 (6)	0.0190 (6)	0.0181 (6)	0.0007 (5)	−0.0004 (5)	0.0013 (5)
C6	0.0180 (6)	0.0158 (6)	0.0136 (5)	0.0005 (4)	0.0013 (4)	0.0001 (4)
C7	0.0164 (6)	0.0166 (6)	0.0160 (6)	−0.0012 (4)	0.0004 (4)	−0.0004 (4)
C8	0.0157 (6)	0.0161 (6)	0.0187 (6)	−0.0021 (4)	−0.0016 (5)	−0.0009 (4)
C9	0.0169 (6)	0.0161 (6)	0.0170 (6)	−0.0007 (5)	0.0003 (5)	0.0006 (4)
C10	0.0168 (6)	0.0148 (5)	0.0147 (6)	0.0006 (4)	0.0002 (4)	−0.0001 (4)
C11	0.0186 (6)	0.0142 (5)	0.0189 (6)	−0.0019 (5)	−0.0004 (5)	−0.0004 (4)
C12	0.0151 (6)	0.0182 (6)	0.0181 (6)	−0.0015 (4)	−0.0015 (5)	−0.0002 (4)
C13	0.0172 (6)	0.0160 (6)	0.0142 (5)	0.0033 (4)	0.0004 (4)	0.0006 (4)
C14	0.0211 (6)	0.0136 (5)	0.0176 (6)	−0.0007 (5)	−0.0010 (5)	−0.0008 (4)
C15	0.0160 (6)	0.0170 (6)	0.0183 (6)	−0.0018 (4)	−0.0024 (5)	0.0001 (4)

Geometric parameters (Å, º)

O1—C9	1.2268 (15)	C7—C8	1.3389 (17)
O2—N1	1.2289 (14)	C7—H7	0.95
O3—N1	1.2331 (14)	C8—C9	1.4795 (16)
N1—C13	1.4708 (15)	C8—H8	0.95
C1—C2	1.3893 (17)	C9—C10	1.5060 (16)
C1—C6	1.4014 (17)	C10—C11	1.3951 (17)
C1—H1	0.95	C10—C15	1.4000 (16)
C2—C3	1.3851 (18)	C11—C12	1.3920 (17)
C2—H2	0.95	C11—H11	0.95
C3—C4	1.3923 (18)	C12—C13	1.3835 (17)
C3—H3	0.95	C12—H12	0.95
C4—C5	1.3885 (17)	C13—C14	1.3850 (17)
C4—H4	0.95	C14—C15	1.3808 (16)
C5—C6	1.4009 (17)	C14—H14	0.95
C5—H5	0.95	C15—H15	0.95
C6—C7	1.4624 (16)		
O2—N1—O3	123.31 (10)	C7—C8—C9	119.15 (11)
O2—N1—C13	118.46 (10)	C7—C8—H8	120.4
O3—N1—C13	118.23 (10)	C9—C8—H8	120.4
C2—C1—C6	120.54 (11)	O1—C9—C8	121.21 (11)
C2—C1—H1	119.7	O1—C9—C10	118.58 (11)
C6—C1—H1	119.7	C8—C9—C10	120.21 (10)

C3—C2—C1	119.95 (11)	C11—C10—C15	119.50 (11)
C3—C2—H2	120.0	C11—C10—C9	123.39 (11)
C1—C2—H2	120.0	C15—C10—C9	117.09 (11)
C2—C3—C4	120.28 (11)	C12—C11—C10	120.40 (11)
C2—C3—H3	119.9	C12—C11—H11	119.8
C4—C3—H3	119.9	C10—C11—H11	119.8
C5—C4—C3	119.93 (11)	C13—C12—C11	118.21 (11)
C5—C4—H4	120.0	C13—C12—H12	120.9
C3—C4—H4	120.0	C11—C12—H12	120.9
C4—C5—C6	120.44 (11)	C12—C13—C14	122.88 (11)
C4—C5—H5	119.8	C12—C13—N1	119.33 (11)
C6—C5—H5	119.8	C14—C13—N1	117.79 (10)
C5—C6—C1	118.85 (11)	C15—C14—C13	118.19 (11)
C5—C6—C7	123.37 (11)	C15—C14—H14	120.9
C1—C6—C7	117.77 (11)	C13—C14—H14	120.9
C8—C7—C6	127.53 (11)	C14—C15—C10	120.80 (11)
C8—C7—H7	116.2	C14—C15—H15	119.6
C6—C7—H7	116.2	C10—C15—H15	119.6

C6—C1—C2—C3	0.74 (19)	C8—C9—C10—C15	175.96 (10)
C1—C2—C3—C4	−0.36 (19)	C15—C10—C11—C12	0.67 (18)
C2—C3—C4—C5	−0.20 (19)	C9—C10—C11—C12	−177.52 (11)
C3—C4—C5—C6	0.38 (18)	C10—C11—C12—C13	0.57 (18)
C4—C5—C6—C1	0.00 (18)	C11—C12—C13—C14	−1.58 (18)
C4—C5—C6—C7	−179.43 (11)	C11—C12—C13—N1	178.29 (10)
C2—C1—C6—C5	−0.56 (18)	O2—N1—C13—C12	−169.34 (11)
C2—C1—C6—C7	178.91 (11)	O3—N1—C13—C12	10.81 (16)
C5—C6—C7—C8	8.14 (19)	O2—N1—C13—C14	10.54 (16)
C1—C6—C7—C8	−171.29 (12)	O3—N1—C13—C14	−169.31 (11)
C6—C7—C8—C9	179.69 (11)	C12—C13—C14—C15	1.28 (18)
C7—C8—C9—O1	0.54 (18)	N1—C13—C14—C15	−178.59 (10)
C7—C8—C9—C10	−179.81 (11)	C13—C14—C15—C10	0.04 (17)
O1—C9—C10—C11	173.86 (12)	C11—C10—C15—C14	−0.99 (18)
C8—C9—C10—C11	−5.80 (17)	C9—C10—C15—C14	177.32 (11)
O1—C9—C10—C15	−4.38 (17)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C1—H1···O1^{i}	0.95	2.47	3.3314 (15)	150
C5—H5···O3^{ii}	0.95	2.56	3.4635 (16)	160

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*+2, *y*+1/2, −*z*+1/2.