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(2*E*,4*E*)-1-(3-Nitrophenyl)-5-phenylpenta-2,4-dien-1-one

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Key indicators

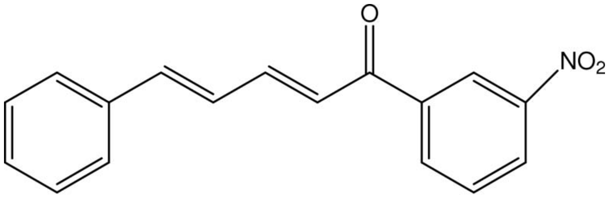
Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.042
wR factor = 0.115
Data-to-parameter ratio = 18.5

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

In the title compound, $C_{17}H_{13}NO_3$, the dihedral angle between the benzene rings is 2.57 (4)°. The crystal structure is stabilized by C—H···O interactions, which form a three-dimensional network, and by C—H···π interactions.

Comment

Lasers are used increasingly for high-speed recording, storage, information transmission and processing. Many electro-optical devices rely on the use of non-linear optical (NLO) materials, in particular those with the capability of frequency conversion (second-harmonic generation, SHG) (Chemla & Zyss, 1987). Among several organic compounds reported for their NLO properties, chalcone derivatives are prominent materials due to their excellent blue-light transmittance and ease of forming crystals. They provide the configuration necessary to show NLO activity, with two planar rings connected through a conjugated double bond (Patil, Teh *et al.*, 2006; Patil, Ng *et al.*, 2007; Patil, Rosli *et al.*, 2007). The title compound, (I), was prepared as part of our ongoing studies on non-linear optical materials (Patil, Dharmaprakash *et al.*, 2006; Shettigar *et al.*, 2006; Chantrapromma, Jindawong *et al.*, 2006; Chantrapromma, Ruanwas *et al.*, 2006). Crystals of the title compound, (I) (Fig. 1), should exhibit second-order NLO properties as they crystallize in a non-centrosymmetric space group.



(I)

Bond lengths and angles in (I) have normal values (Allen *et al.*, 1987). The least-squares plane through the C7–C11/O1

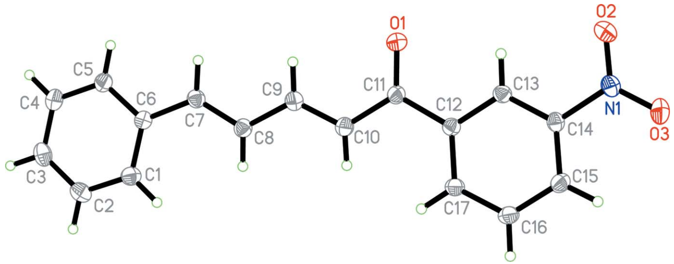


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom numbering.

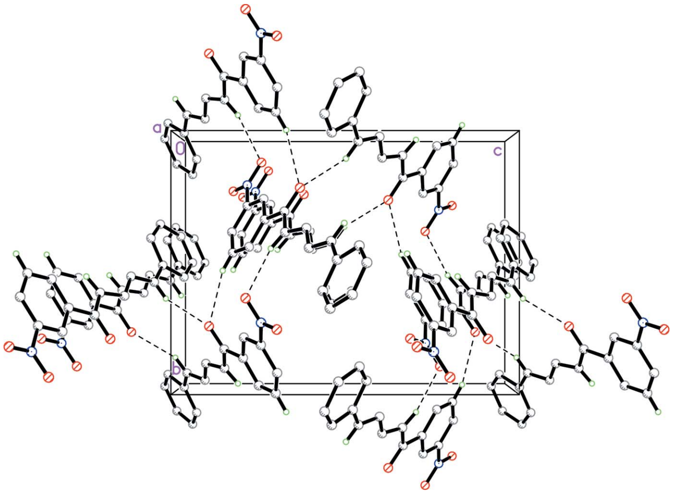


Figure 2
The crystal packing of (I), viewed down the *a* axis. Dashed lines indicate hydrogen bonds. H atoms not involved in hydrogen bonding have been omitted for clarity.

group makes dihedral angles of 7.04 (4) and 8.70 (4)° with the C1–C6 and C12–C17 benzene rings, respectively. The dihedral angle between these rings is 2.57 (4)° and the nitro group at C14 lies close to the C12–C17 ring plane, with O2—N1—C14—C13 and O3—N1—C14—C15 torsion angles of 0.17 (18) and 1.60 (19)°, respectively.

The crystal structure (Fig. 2) is stabilized by C—H···O interactions (Table 1), which form a three-dimensional network, and is further consolidated by C—H···π interactions (Table 1) involving the C1–C6 benzene ring.

Experimental

Cinnamaldehyde (0.01 mol) and 3-nitroacetophenone (0.01 mol) were stirred in methanol (60 ml) at room temperature. 10% aqueous NaOH solution (5 g) was added and the mixture stirred for 2 h. The resulting precipitate was filtered, washed with water, dried and the crude product recrystallized from acetone. Crystals suitable for X-ray analysis were grown by slow evaporation of an acetone solution at room temperature.

Crystal data

$C_{17}H_{13}NO_3$
$M_r = 279.28$
Orthorhombic, $P2_12_12_1$
$a = 7.0167$ (1) Å
$b = 12.1953$ (2) Å
$c = 16.1081$ (3) Å
$V = 1378.38$ (4) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 100.0$ (1) K
0.47 × 0.26 × 0.14 mm

Data collection

Bruker SMART APEX2 CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
$T_{\rm min} = 0.864$, $T_{\rm max} = 0.988$
38028 measured reflections
3523 independent reflections
3097 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.044$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.115$
$S = 1.07$
3523 reflections
190 parameters
H-atom parameters constrained
$\Delta\rho_{\rm max} = 0.29$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.21$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7A···O1$^{\rm i}$	0.93	2.42	3.297 (2)	157
C10—H10A···O2$^{\rm ii}$	0.93	2.47	3.358 (2)	159
C16—H16A···O1$^{\rm ii}$	0.93	2.57	3.462 (2)	161
C15—H15A···$Cg1^{\rm iii}$	0.93	2.76	3.612 (1)	152

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{3}{2}, -z$; (ii) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, -y+2, z+\frac{1}{2}$. $Cg1$ is the centroid of the C1–C6 ring.

In the absence of significant anomalous scattering effects, 2727 Friedel pairs were merged. H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å and $U_{\rm iso}({\rm H}) = 1.2U_{\rm eq}({\rm C})$.

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

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Acta Cryst. (2007). E**63**, o2122–o2123 Patil *et al.* • $C_{17}H_{13}NO_3$ **o2123**