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(2*E*)-3-[4-(Dimethylamino)phenyl]-1-(3-nitrophenyl)prop-2-en-1-one

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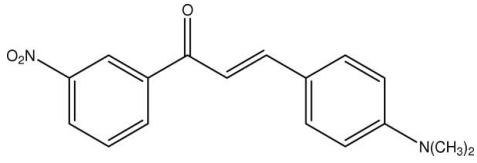
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.054; wR factor = 0.162; data-to-parameter ratio = 20.6.

In the title compound, $C_{17}H_{16}N_2O_3$, the dihedral angle between the benzene rings is 1.56 (7)°. The nitro group is coplanar with the attached benzene ring while the dimethylamino group is twisted slightly away from the attached benzene ring. A weak intramolecular C—H···O hydrogen bond is present in the molecular structure. The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds, forming chains along the [011] direction.

Related literature

For bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For general background and related literature, see: Uchida *et al.* (1998); Watson *et al.* (1993); Patil, Dharmaprakash *et al.* (2006); Shettigar *et al.* (2006).



Experimental

Crystal data

$C_{17}H_{16}N_2O_3$
M_r = 296.32
Triclinic, $P\overline{1}$
a = 6.4326 (2) Å
b = 7.1724 (2) Å
c = 16.5000 (6) Å
α = 93.989 (2)°
β = 96.973 (2)°
γ = 107.844 (2)°
V = 714.68 (4) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 100.0 (1) K
0.58 × 0.25 × 0.04 mm

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.822, T_{max} = 0.996
12950 measured reflections
4139 independent reflections
2776 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.162
S = 1.07
4139 reflections
201 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.33 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H9A···O1	0.93	2.45	2.798 (2)	102
C17—H17C···O3^{i}	0.96	2.59	3.430 (2)	146

Symmetry code: (i) $x, y-1, z-1$.

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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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2370).

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supplementary materials

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(2*E*)-3-[4-(Dimethylamino)phenyl]-1-(3-nitrophenyl)prop-2-en-1-one

M. M. Rosli, P. S. Patil, H.-K. Fun, I. A. Razak and S. M. Dharmaprakash

Comment

Many chalcone derivatives crystallize as noncentrosymmetric structures and display significant non-linear optical (NLO) properties (Uchida *et al.*, 1998; Patil *et al.*, 2006; Shettigar *et al.*, 2006). Crystals of the title compound, (I), do not exhibit second-order NLO properties, as the compound crystallizes in a centrosymmetric space group (Watson *et al.*, 1993).

Bond lengths and angles in (I) (Fig. 1) have normal values (Allen *et al.*, 1987). The dihedral angle between the benzene rings is 1.56 (7)°. The plane through the enone group (O1/C7—C9) makes dihedral angles of 10.47 (7) and 9.23 (7)°, respectively, with the C1—C6 and C10—C15 benzene rings. The nitro group attached at atom C2 is almost coplanar with the C1—C6 benzene ring, with torsion angles O2–N2–C2–C1 and O3–N2–C2–C3 of -2.5 (2)° and -2.1 (2)°, respectively. The dimethylamino group is twisted slightly away from the attached C10—C15 benzene ring, with torsion angles C16–N1–C13–C14 and C17–N1–C13–C12 of 10.5 (2)° and -8.3 (2)°, respectively.

An intramolecular C9—H9A···O1 interaction is observed in the molecular structure of (I), and it generates an S(5) ring motif (Bernstein *et al.*, 1995). The molecules are linked into a chain along the [0 1 1] direction by intermolecular C17—H17C···O3^{i} hydrogen bonds (Table 1). In addition, π-π interactions involving the C1—C6 (centroid Cg1) and C10—C15 (centroid Cg2) benzene rings is observed, with a Cg1···Cg2^{ii} distance of 3.5164 (8) Å. Symmetry codes: (i) x,-1+y,-1+z; (ii) 1-x, -y, 1-z.

Experimental

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

Refinement

All H atoms were refined using a riding model, with C—H distances in the range 0.93-0.96 Å. The U_{iso}(H) values were constrained to be 1.5U_{eq} of the carrier atom for methyl H and 1.2U_{eq} for the remaining H atoms.

Figures

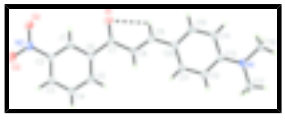
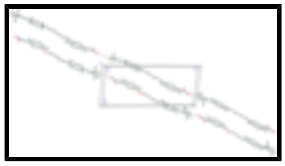


Figure 1 The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The dashed line indicates a hydrogen bond.
Figure 2 The crystal packing of (I), viewed down the *a* axis. Hydrogen bonds are shown as dashed lines.



(2E)-3-[4-(dimethylamino)phenyl]-1-(3-nitrophenyl) prop-2-en-1-one

Crystal data

$C_{17}H_{16}N_2O_3$	$Z = 2$
$M_r = 296.32$	$F_{000} = 312$
Triclinic, $P\bar{1}$	$D_x = 1.377$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 6.4326$ (2) Å	Cell parameters from 2515 reflections
$b = 7.1724$ (2) Å	$\theta = 3.0$–30.0º
$c = 16.5000$ (6) Å	$\mu = 0.10$ mm^{-1}
$\alpha = 93.989$ (2)º	$T = 100.0$ (1) K
$\beta = 96.973$ (2)º	Plate, red
$\gamma = 107.844$ (2)º	0.58 × 0.25 × 0.04 mm
$V = 714.68$ (4) Å^3	

Data collection

Bruker SMART APEX2 CCD area-detector diffractometer	4139 independent reflections
Radiation source: fine-focus sealed tube	2776 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.047$
Detector resolution: 8.33 pixels mm^{-1}	$\theta_{max} = 30.0$º
$T = 100.0(1)$ K	$\theta_{min} = 1.3$º
ω scans	$h = -9 \rightarrow 9$
Absorption correction: multi-scan (SADABS; Bruker, 2005)	$k = -10 \rightarrow 10$
$T_{min} = 0.822$, $T_{max} = 0.996$	$l = -23 \rightarrow 22$
12950 measured reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0746P)^2 + 0.1229P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.054$	$(\Delta/\sigma)_{max} = 0.001$
$wR(F^2) = 0.162$	$\Delta\rho_{max} = 0.31$ e Å^{-3}
$S = 1.07$	$\Delta\rho_{min} = -0.33$ e Å^{-3}
4139 reflections	Extinction correction: none
201 parameters	

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

Special details

Experimental. The data was collected with the Oxford Cyrosystem Cobra low-temperature attachment.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 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 ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.20474 (19)	0.31302 (18)	0.58398 (7)	0.0307 (3)
O2	0.4006 (2)	0.58466 (19)	0.86676 (8)	0.0358 (3)
O3	0.7425 (2)	0.7068 (2)	0.92259 (7)	0.0403 (3)
N1	0.3580 (2)	−0.16780 (19)	0.12184 (8)	0.0242 (3)
N2	0.5992 (2)	0.6233 (2)	0.86426 (8)	0.0268 (3)
C1	0.5108 (3)	0.4710 (2)	0.72163 (9)	0.0208 (3)
H1A	0.3618	0.4382	0.7267	0.025*
C2	0.6705 (3)	0.5694 (2)	0.78695 (9)	0.0214 (3)
C3	0.8939 (3)	0.6208 (2)	0.78275 (10)	0.0240 (3)
H3A	0.9984	0.6875	0.8278	0.029*
C4	0.9570 (3)	0.5698 (2)	0.70954 (10)	0.0241 (3)
H4A	1.1064	0.6022	0.7051	0.029*
C5	0.8002 (3)	0.4708 (2)	0.64249 (10)	0.0219 (3)
H5A	0.8458	0.4373	0.5937	0.026*
C6	0.5761 (2)	0.4212 (2)	0.64736 (9)	0.0193 (3)
C7	0.3950 (3)	0.3212 (2)	0.57715 (9)	0.0210 (3)
C8	0.4516 (3)	0.2383 (2)	0.50196 (9)	0.0214 (3)
H8A	0.5986	0.2544	0.4973	0.026*
C9	0.2920 (3)	0.1398 (2)	0.44018 (9)	0.0215 (3)
H9A	0.1479	0.1214	0.4497	0.026*
C10	0.3166 (3)	0.0582 (2)	0.36015 (9)	0.0199 (3)
C11	0.5214 (3)	0.0810 (2)	0.33381 (9)	0.0211 (3)
H11A	0.6505	0.1461	0.3699	0.025*
C12	0.5359 (3)	0.0091 (2)	0.25577 (9)	0.0214 (3)
H12A	0.6743	0.0273	0.2401	0.026*
C13	0.3440 (3)	−0.0919 (2)	0.19893 (9)	0.0205 (3)
C14	0.1394 (3)	−0.1144 (2)	0.22557 (9)	0.0228 (3)

H14A	0.0099	−0.1794	0.1898	0.027*
C15	0.1271 (3)	−0.0417 (2)	0.30389 (9)	0.0222 (3)
H15A	−0.0110	−0.0596	0.3197	0.027*
C16	0.1605 (3)	−0.2440 (3)	0.06120 (10)	0.0302 (4)
H16A	0.0543	−0.3489	0.0816	0.045*
H16B	0.1976	−0.2932	0.0112	0.045*
H16C	0.0988	−0.1404	0.0507	0.045*
C17	0.5695 (3)	−0.1231 (3)	0.09321 (11)	0.0336 (4)
H17A	0.6665	−0.1716	0.1284	0.050*
H17B	0.6326	0.0170	0.0941	0.050*
H17C	0.5499	−0.1850	0.0381	0.050*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0225 (6)	0.0426 (7)	0.0256 (6)	0.0097 (5)	0.0054 (5)	−0.0044 (5)
O2	0.0301 (7)	0.0514 (8)	0.0276 (7)	0.0160 (6)	0.0078 (5)	−0.0043 (5)
O3	0.0400 (8)	0.0535 (8)	0.0233 (7)	0.0158 (6)	−0.0023 (6)	−0.0142 (6)
N1	0.0239 (7)	0.0293 (7)	0.0180 (7)	0.0086 (5)	0.0007 (5)	−0.0030 (5)
N2	0.0304 (8)	0.0307 (7)	0.0209 (7)	0.0136 (6)	0.0032 (6)	−0.0023 (5)
C1	0.0224 (8)	0.0197 (7)	0.0220 (8)	0.0091 (6)	0.0042 (6)	0.0016 (5)
C2	0.0273 (8)	0.0209 (7)	0.0188 (7)	0.0115 (6)	0.0056 (6)	0.0005 (5)
C3	0.0259 (8)	0.0201 (7)	0.0241 (8)	0.0069 (6)	−0.0009 (6)	−0.0006 (6)
C4	0.0198 (8)	0.0220 (7)	0.0305 (9)	0.0068 (6)	0.0047 (6)	0.0018 (6)
C5	0.0246 (8)	0.0205 (7)	0.0233 (8)	0.0097 (6)	0.0077 (6)	0.0025 (6)
C6	0.0231 (8)	0.0161 (6)	0.0199 (7)	0.0076 (6)	0.0044 (6)	0.0026 (5)
C7	0.0238 (8)	0.0200 (7)	0.0197 (7)	0.0072 (6)	0.0055 (6)	0.0013 (5)
C8	0.0228 (8)	0.0221 (7)	0.0206 (8)	0.0087 (6)	0.0049 (6)	0.0006 (5)
C9	0.0248 (8)	0.0200 (7)	0.0217 (8)	0.0090 (6)	0.0059 (6)	0.0029 (6)
C10	0.0249 (8)	0.0167 (6)	0.0186 (7)	0.0076 (6)	0.0027 (6)	0.0015 (5)
C11	0.0220 (8)	0.0196 (7)	0.0198 (7)	0.0058 (6)	0.0000 (6)	−0.0006 (5)
C12	0.0209 (7)	0.0221 (7)	0.0212 (8)	0.0071 (6)	0.0035 (6)	0.0004 (6)
C13	0.0260 (8)	0.0172 (6)	0.0185 (7)	0.0082 (6)	0.0019 (6)	0.0000 (5)
C14	0.0228 (8)	0.0211 (7)	0.0221 (8)	0.0060 (6)	−0.0016 (6)	−0.0009 (6)
C15	0.0220 (8)	0.0225 (7)	0.0230 (8)	0.0081 (6)	0.0039 (6)	0.0027 (6)
C16	0.0315 (9)	0.0332 (9)	0.0209 (8)	0.0065 (7)	−0.0012 (7)	−0.0037 (6)
C17	0.0308 (9)	0.0447 (10)	0.0243 (9)	0.0125 (8)	0.0054 (7)	−0.0061 (7)

Geometric parameters (Å, °)

O1—C7	1.2268 (18)	C8—H8A	0.93
O2—N2	1.2282 (18)	C9—C10	1.453 (2)
O3—N2	1.2253 (18)	C9—H9A	0.93
N1—C13	1.3726 (19)	C10—C15	1.400 (2)
N1—C17	1.445 (2)	C10—C11	1.403 (2)
N1—C16	1.450 (2)	C11—C12	1.378 (2)
N2—C2	1.4728 (19)	C11—H11A	0.93
C1—C2	1.377 (2)	C12—C13	1.416 (2)
C1—C6	1.401 (2)	C12—H12A	0.93

C1—H1A	0.93	C13—C14	1.404 (2)
C2—C3	1.382 (2)	C14—C15	1.380 (2)
C3—C4	1.380 (2)	C14—H14A	0.93
C3—H3A	0.93	C15—H15A	0.93
C4—C5	1.388 (2)	C16—H16A	0.96
C4—H4A	0.93	C16—H16B	0.96
C5—C6	1.389 (2)	C16—H16C	0.96
C5—H5A	0.93	C17—H17A	0.96
C6—C7	1.503 (2)	C17—H17B	0.96
C7—C8	1.471 (2)	C17—H17C	0.96
C8—C9	1.339 (2)		
C13—N1—C17	120.03 (13)	C10—C9—H9A	116.0
C13—N1—C16	119.75 (13)	C15—C10—C11	117.16 (13)
C17—N1—C16	117.94 (13)	C15—C10—C9	119.05 (14)
O3—N2—O2	123.47 (14)	C11—C10—C9	123.73 (14)
O3—N2—C2	117.85 (14)	C12—C11—C10	121.55 (14)
O2—N2—C2	118.67 (13)	C12—C11—H11A	119.2
C2—C1—C6	118.98 (14)	C10—C11—H11A	119.2
C2—C1—H1A	120.5	C11—C12—C13	121.21 (14)
C6—C1—H1A	120.5	C11—C12—H12A	119.4
C1—C2—C3	122.83 (14)	C13—C12—H12A	119.4
C1—C2—N2	118.35 (14)	N1—C13—C14	121.62 (14)
C3—C2—N2	118.82 (14)	N1—C13—C12	121.33 (14)
C4—C3—C2	117.84 (15)	C14—C13—C12	117.04 (13)
C4—C3—H3A	121.1	C15—C14—C13	121.22 (14)
C2—C3—H3A	121.1	C15—C14—H14A	119.4
C3—C4—C5	120.78 (15)	C13—C14—H14A	119.4
C3—C4—H4A	119.6	C14—C15—C10	121.82 (14)
C5—C4—H4A	119.6	C14—C15—H15A	119.1
C4—C5—C6	120.80 (14)	C10—C15—H15A	119.1
C4—C5—H5A	119.6	N1—C16—H16A	109.5
C6—C5—H5A	119.6	N1—C16—H16B	109.5
C5—C6—C1	118.76 (14)	H16A—C16—H16B	109.5
C5—C6—C7	124.49 (13)	N1—C16—H16C	109.5
C1—C6—C7	116.73 (13)	H16A—C16—H16C	109.5
O1—C7—C8	122.01 (14)	H16B—C16—H16C	109.5
O1—C7—C6	118.94 (13)	N1—C17—H17A	109.5
C8—C7—C6	119.04 (13)	N1—C17—H17B	109.5
C9—C8—C7	120.16 (14)	H17A—C17—H17B	109.5
C9—C8—H8A	119.9	N1—C17—H17C	109.5
C7—C8—H8A	119.9	H17A—C17—H17C	109.5
C8—C9—C10	127.92 (15)	H17B—C17—H17C	109.5
C8—C9—H9A	116.0		
C6—C1—C2—C3	−0.4 (2)	C6—C7—C8—C9	176.63 (13)
C6—C1—C2—N2	179.16 (12)	C7—C8—C9—C10	176.15 (14)
O3—N2—C2—C1	178.37 (14)	C8—C9—C10—C15	179.55 (14)
O2—N2—C2—C1	−2.5 (2)	C8—C9—C10—C11	−3.4 (2)
O3—N2—C2—C3	−2.1 (2)	C15—C10—C11—C12	0.3 (2)

O2—N2—C2—C3	177.06 (14)	C9—C10—C11—C12	−176.72 (14)
C1—C2—C3—C4	−0.1 (2)	C10—C11—C12—C13	−0.3 (2)
N2—C2—C3—C4	−179.64 (13)	C17—N1—C13—C14	173.04 (14)
C2—C3—C4—C5	0.2 (2)	C16—N1—C13—C14	10.5 (2)
C3—C4—C5—C6	0.2 (2)	C17—N1—C13—C12	−8.3 (2)
C4—C5—C6—C1	−0.7 (2)	C16—N1—C13—C12	−170.82 (13)
C4—C5—C6—C7	177.56 (13)	C11—C12—C13—N1	−178.40 (13)
C2—C1—C6—C5	0.7 (2)	C11—C12—C13—C14	0.3 (2)
C2—C1—C6—C7	−177.63 (12)	N1—C13—C14—C15	178.41 (13)
C5—C6—C7—O1	−168.19 (14)	C12—C13—C14—C15	−0.3 (2)
C1—C6—C7—O1	10.1 (2)	C13—C14—C15—C10	0.3 (2)
C5—C6—C7—C8	11.0 (2)	C11—C10—C15—C14	−0.3 (2)
C1—C6—C7—C8	−170.71 (12)	C9—C10—C15—C14	176.88 (13)
O1—C7—C8—C9	−4.2 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H9A···O1	0.93	2.45	2.798 (2)	102
C17—H17C···O3^{i}	0.96	2.59	3.430 (2)	146

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

Fig. 1

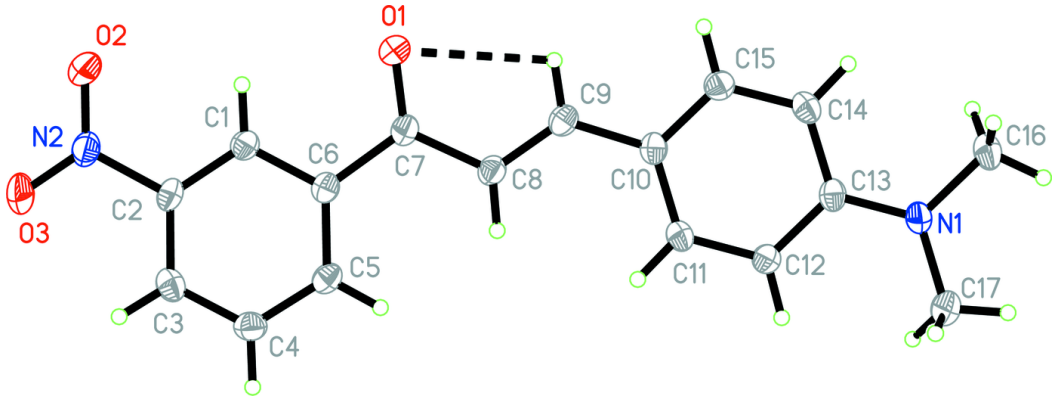

O1
O2
N2
O3
C1
C2
C3
C4
C5
C6
C7
C8
C9
C10
C11
C12
C13
C14
C15
C16
C17
N1

Fig. 2