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N-(4-Nitrophenyl)cinnamamide

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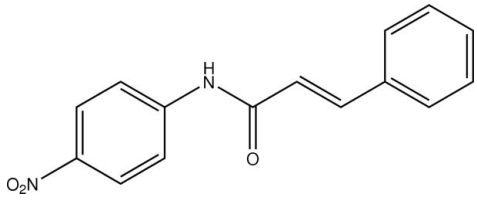
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.043; wR factor = 0.117; data-to-parameter ratio = 15.9.

In the molecule of the title compound, $C_{15}H_{12}N_2O_3$, the dihedral angle between the rings is 3.04 (8)°. The central NOC_3 fragment is planar [maximum deviation = 0.005 (3) Å] and is oriented at dihedral angles of 8.23 (8) and 7.29 (9)° with respect to the phenyl and nitrophenyl rings, respectively. In the crystal structure, intermolecular N—H···O and C—H···O interactions link the molecules into a two-dimensional network. π–π contacts between rings [centroid–centroid distance = 3.719 (1) Å] may further stabilize the structure.

Related literature

For general background to *N*-substituted benzamides, see: Beccalli *et al.* (2005); Calderone *et al.* (2006); Lindgren *et al.* (2001); Olsson *et al.* (2002); Vega-Noverola *et al.* (1989); Zhichkin *et al.* (2007). For related structures, see: Nissa *et al.* (2002, 2004); Peeters *et al.* (1986). For a description of the Cambridge Structural Database, see: Allen (2002).



Experimental

Crystal data

$C_{15}H_{12}N_2O_3$
M_r = 268.27
Monoclinic, $P2_1/c$
a = 5.903 (3) Å
b = 15.050 (9) Å
c = 14.388 (9) Å
β = 95.38 (3)°
V = 1272.6 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 173 K
0.20 × 0.18 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.980, T_{max} = 0.984
10408 measured reflections
2886 independent reflections
1994 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.117
S = 1.07
2886 reflections
181 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.88	2.13	2.991 (2)	166
C5—H5···O2^{ii}	0.95	2.58	3.519 (2)	168

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, y+1, z$.

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DENZO* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* (Otwinowski & Minor, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2746).

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N-(4-Nitrophenyl)cinnamamide

Aamer Saeed, Rasheed Ahmad Khera, Muhammad Shahid and Masood Parvez

S1. Comment

N-substituted benzamides, *e.g.*, declopramideare, are well known anticancer compounds and the mechanism of benzamide-induced apoptosis has been studied, (Olsson *et al.*, 2002). N-substituted benzamides inhibit the activity of nuclear factor-B and nuclear factor of activated T cells (Lindgren *et al.*, 2001). Various N-substituted benzamides exhibit potent antiemetic activity (Vega-Noverola *et al.*, 1989), while heterocyclic benzanilide are potassium channel activators (Calderone *et al.*, 2006). *N*-Alkylated 2-nitrobenzamides are intermediates in the synthesis of dibenzo[b,e][1,4]diazepines (Zhichkin *et al.*, 2007) and *N*-Acyl-2-nitrobenzamides are precursors of 2,3-disubstitued 3*H*-quinazoline-4-ones (Beccalli *et al.*, 2005). As part of our work on the structure of benzanilides and related compounds, we report herein the crystal structure of the title compound.

A search of the Cambridge Crystallographic Database (CSD version 5.30; Allen, 2002) for a fragment containing the title compound without NO_2 group revealed only four entries containg the basic skeleton of the title compound with refcodes: DIPHUF (Peeters *et al.*, 1986), EHATUC and EHAVAK (Nissa *et al.*, 2002) and FALQAL (Nissa *et al.*, 2004).

In the molecule of the title compound (Fig. 1), rings A (C1-C6) and B (C10-C15) are, of course, planar and they are oriented at a dihedral angle of A/B = 3.04 (8)°. The (O1/N1/C7-C9) moiety is planar with a maximum deviation of -0.005 (3) Å for atom C8 and it is oriented with respect to rings A and B at dihedral angles of 8.23 (8) and 7.29 (9) °, respectively.

In the crystal structure, intermolecular N-H···O and C-H···O interactions (Table 1) link the molecules into a two dimensional network (Fig. 2), in which they may be effective in the stabilization of the structure. The *π*–*π* contact between the phenyl rings, Cg1—Cg2^{i} [symmetry code: (i) 1 - x, y - 1/2, 1/2 - z, where Cg1 and Cg2 are centroids of the rings A (C1-C6) and B (C10-C15), respectively] may further stabilize the structure, with centroid-centroid distance of 3.719 (1) Å.

S2. Experimental

For the preparation of the title compound, cinnamic acid was converted into cinnamoyl chloride using the standard procedure. A stirred solution of cinnamoyl chloride (5.4 mmol) in $CHCl_3$ was treated with *p*-nitroaniline (21.6 mmol) under a nitrogen atmosphere at reflux for 4 h. Upon cooling, the reaction mixture was diluted with $CHCl_3$ and washed consecutively with aq 1.0 *M* HCl and saturated aq $NaHCO_3$. The organic layer was dried over anhydrous magnesium sulfate and concentrated under reduced pressure. Crystallization of the residue in MeOH afforded the title compound (yield; 81%) as colorless crystals: Anal. calcd. for $C_{15}H_{12}N_2O_3$: C, 67.16; H, 4.51; N, 10.44; found: C, 67.21; H, 4.59; N, 10.41.

S3. Refinement

H atoms were positioned geometrically with N-H = 0.88 Å (for NH) and C-H = 0.95 Å for aromatic H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,N).

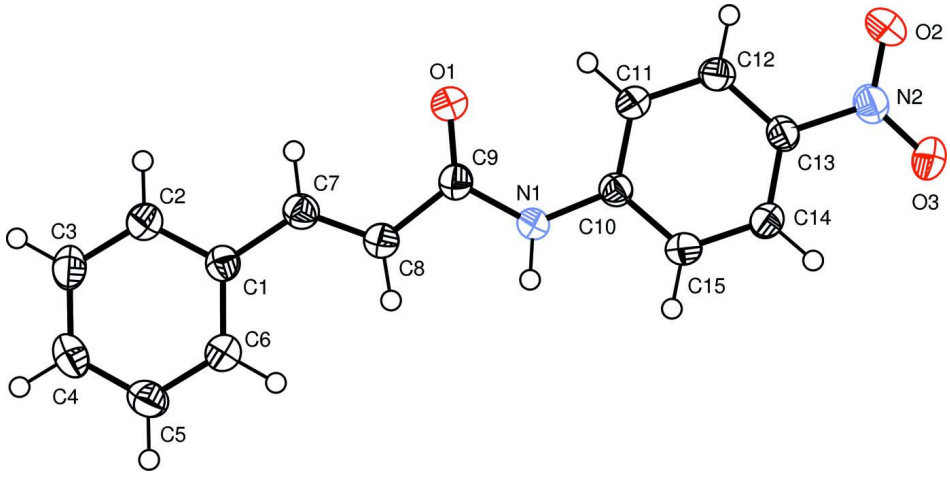

Figure 1

The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level

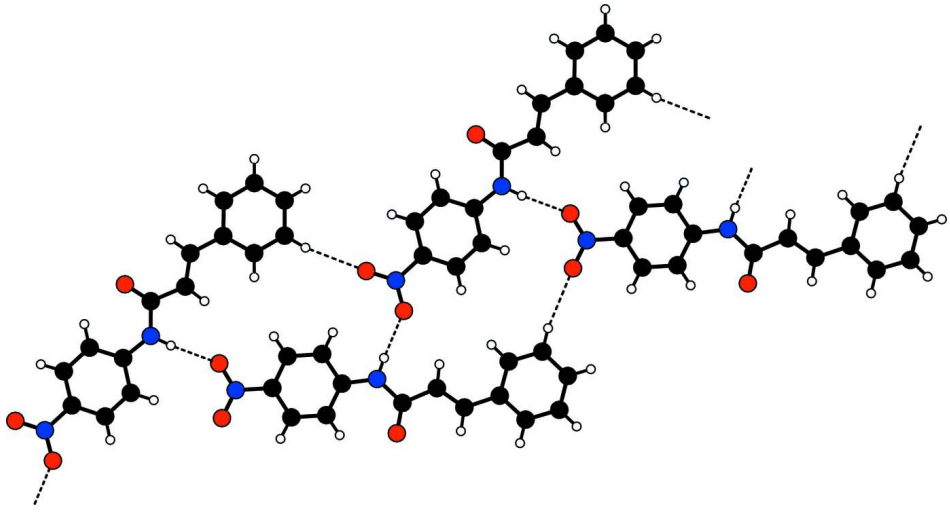

Figure 2

A partial packing diagram. Hydrogen bonds are shown as dashed lines.

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Crystal data

$C_{15}H_{12}N_2O_3$
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Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 5.903 (3) Å
b = 15.050 (9) Å
c = 14.388 (9) Å
β = 95.38 (3)°
V = 1272.6 (13) Å^3
Z = 4
F(000) = 560
D_x = 1.400 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 10408 reflections

θ = 3.1–27.4°
μ = 0.10 mm^{-1}
T = 173 K

Block, colorless
0.20 × 0.18 × 0.16 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1997)
T_{min} = 0.980, T_{max} = 0.984

10408 measured reflections
2886 independent reflections
1994 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 27.4°, θ_{min} = 3.1°
h = −7→7
k = −18→19
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.117
S = 1.07
2886 reflections
181 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
$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.2254P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.73930 (18)	0.43225 (7)	0.92756 (8)	0.0419 (3)
O2	0.2344 (2)	0.02701 (7)	0.81198 (8)	0.0477 (3)
O3	−0.0962 (2)	0.07667 (8)	0.75877 (9)	0.0534 (4)
N1	0.3863 (2)	0.44089 (8)	0.84727 (9)	0.0327 (3)
H1	0.2850	0.4794	0.8233	0.039*
N2	0.1031 (2)	0.08866 (8)	0.79176 (9)	0.0368 (3)
C1	0.7780 (2)	0.71883 (10)	0.93224 (10)	0.0299 (3)
C2	0.9858 (3)	0.75660 (11)	0.96491 (10)	0.0355 (4)
H2	1.1095	0.7191	0.9862	0.043*
C3	1.0150 (3)	0.84803 (11)	0.96685 (11)	0.0416 (4)
H3	1.1580	0.8727	0.9892	0.050*
C4	0.8371 (3)	0.90315 (11)	0.93650 (11)	0.0415 (4)
H4	0.8574	0.9658	0.9375	0.050*

C5	0.6279 (3)	0.86698 (11)	0.90433 (11)	0.0401 (4)
H5	0.5047	0.9048	0.8835	0.048*
C6	0.5991 (3)	0.77560 (10)	0.90259 (10)	0.0346 (4)
H6	0.4553	0.7513	0.8809	0.041*
C7	0.7580 (2)	0.62167 (10)	0.92964 (10)	0.0316 (4)
H7	0.8827	0.5887	0.9584	0.038*
C8	0.5822 (2)	0.57539 (10)	0.89084 (10)	0.0334 (4)
H8	0.4535	0.6061	0.8621	0.040*
C9	0.5825 (2)	0.47700 (10)	0.89143 (10)	0.0316 (4)
C10	0.3266 (2)	0.35165 (10)	0.83539 (10)	0.0282 (3)
C11	0.4746 (2)	0.28151 (10)	0.85797 (10)	0.0316 (4)
H11	0.6261	0.2930	0.8834	0.038*
C12	0.4016 (3)	0.19496 (10)	0.84341 (10)	0.0322 (4)
H12	0.5021	0.1467	0.8586	0.039*
C13	0.1807 (2)	0.17939 (9)	0.80651 (10)	0.0300 (3)
C14	0.0315 (2)	0.24827 (10)	0.78241 (10)	0.0323 (4)
H14	−0.1191	0.2362	0.7562	0.039*
C15	0.1037 (2)	0.33422 (10)	0.79678 (10)	0.0315 (3)
H15	0.0026	0.3821	0.7806	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0340 (6)	0.0328 (6)	0.0563 (7)	0.0019 (5)	−0.0103 (5)	−0.0006 (5)
O2	0.0508 (7)	0.0283 (6)	0.0626 (8)	0.0039 (6)	−0.0020 (6)	0.0050 (5)
O3	0.0390 (7)	0.0386 (7)	0.0794 (9)	−0.0086 (5)	−0.0118 (6)	−0.0074 (6)
N1	0.0305 (7)	0.0242 (7)	0.0418 (7)	0.0007 (5)	−0.0051 (5)	0.0016 (6)
N2	0.0403 (8)	0.0300 (7)	0.0397 (8)	−0.0026 (6)	0.0021 (6)	−0.0015 (6)
C1	0.0325 (8)	0.0302 (8)	0.0269 (7)	−0.0008 (6)	0.0027 (6)	−0.0009 (6)
C2	0.0356 (8)	0.0348 (9)	0.0354 (8)	−0.0007 (7)	−0.0012 (6)	−0.0009 (7)
C3	0.0430 (10)	0.0373 (9)	0.0436 (10)	−0.0102 (8)	−0.0009 (7)	−0.0050 (7)
C4	0.0543 (10)	0.0278 (9)	0.0426 (10)	−0.0049 (8)	0.0057 (8)	−0.0017 (7)
C5	0.0453 (10)	0.0328 (9)	0.0420 (9)	0.0059 (8)	0.0024 (7)	0.0025 (7)
C6	0.0328 (8)	0.0346 (9)	0.0358 (8)	−0.0008 (7)	0.0009 (6)	−0.0010 (7)
C7	0.0330 (8)	0.0311 (8)	0.0307 (8)	0.0010 (7)	0.0027 (6)	0.0005 (6)
C8	0.0318 (8)	0.0306 (8)	0.0370 (8)	−0.0003 (7)	−0.0003 (6)	0.0021 (7)
C9	0.0307 (8)	0.0303 (8)	0.0337 (8)	−0.0026 (7)	0.0016 (6)	0.0003 (6)
C10	0.0298 (8)	0.0272 (8)	0.0275 (7)	0.0004 (6)	0.0019 (6)	−0.0002 (6)
C11	0.0282 (8)	0.0311 (8)	0.0344 (8)	0.0008 (6)	−0.0029 (6)	−0.0004 (6)
C12	0.0330 (8)	0.0298 (8)	0.0332 (8)	0.0036 (7)	−0.0009 (6)	0.0001 (6)
C13	0.0329 (8)	0.0248 (7)	0.0322 (8)	−0.0016 (6)	0.0027 (6)	−0.0007 (6)
C14	0.0271 (7)	0.0332 (8)	0.0363 (8)	−0.0016 (7)	0.0013 (6)	−0.0020 (7)
C15	0.0283 (7)	0.0314 (8)	0.0343 (8)	0.0033 (6)	0.0010 (6)	0.0016 (7)

Geometric parameters (Å, º)

O1—C9	1.2207 (18)	C5—H5	0.9500
O2—N2	1.2264 (17)	C6—H6	0.9500

O3—N2	1.2397 (17)	C7—C8	1.329 (2)
N1—C9	1.3790 (19)	C7—H7	0.9500
N1—C10	1.395 (2)	C8—C9	1.481 (2)
N1—H1	0.8800	C8—H8	0.9500
N2—C13	1.450 (2)	C10—C11	1.389 (2)
C1—C2	1.393 (2)	C10—C15	1.404 (2)
C1—C6	1.394 (2)	C11—C12	1.382 (2)
C1—C7	1.467 (2)	C11—H11	0.9500
C2—C3	1.387 (2)	C12—C13	1.381 (2)
C2—H2	0.9500	C12—H12	0.9500
C3—C4	1.377 (2)	C13—C14	1.383 (2)
C3—H3	0.9500	C14—C15	1.372 (2)
C4—C5	1.389 (2)	C14—H14	0.9500
C4—H4	0.9500	C15—H15	0.9500
C5—C6	1.386 (2)		

C9—N1—C10	128.87 (13)	C1—C7—H7	116.9
C9—N1—H1	115.6	C7—C8—C9	121.43 (14)
C10—N1—H1	115.6	C7—C8—H8	119.3
O2—N2—O3	122.46 (13)	C9—C8—H8	119.3
O2—N2—C13	119.59 (13)	O1—C9—N1	123.31 (14)
O3—N2—C13	117.95 (13)	O1—C9—C8	123.67 (14)
C2—C1—C6	118.10 (14)	N1—C9—C8	113.01 (13)
C2—C1—C7	118.78 (14)	C11—C10—N1	123.82 (13)
C6—C1—C7	123.12 (13)	C11—C10—C15	119.74 (14)
C3—C2—C1	121.03 (15)	N1—C10—C15	116.44 (13)
C3—C2—H2	119.5	C12—C11—C10	120.02 (14)
C1—C2—H2	119.5	C12—C11—H11	120.0
C4—C3—C2	120.12 (15)	C10—C11—H11	120.0
C4—C3—H3	119.9	C13—C12—C11	119.22 (14)
C2—C3—H3	119.9	C13—C12—H12	120.4
C3—C4—C5	119.84 (15)	C11—C12—H12	120.4
C3—C4—H4	120.1	C12—C13—C14	121.69 (14)
C5—C4—H4	120.1	C12—C13—N2	119.36 (13)
C6—C5—C4	119.92 (15)	C14—C13—N2	118.95 (14)
C6—C5—H5	120.0	C15—C14—C13	119.18 (14)
C4—C5—H5	120.0	C15—C14—H14	120.4
C5—C6—C1	120.97 (15)	C13—C14—H14	120.4
C5—C6—H6	119.5	C14—C15—C10	120.14 (14)
C1—C6—H6	119.5	C14—C15—H15	119.9
C8—C7—C1	126.22 (14)	C10—C15—H15	119.9
C8—C7—H7	116.9		

C6—C1—C2—C3	−0.8 (2)	C9—N1—C10—C15	172.82 (14)
C7—C1—C2—C3	178.57 (14)	N1—C10—C11—C12	−179.62 (14)
C1—C2—C3—C4	0.2 (2)	C15—C10—C11—C12	−0.7 (2)
C2—C3—C4—C5	0.3 (2)	C10—C11—C12—C13	−0.1 (2)
C3—C4—C5—C6	−0.2 (2)	C11—C12—C13—C14	1.0 (2)

C4—C5—C6—C1	−0.4 (2)	C11—C12—C13—N2	−179.58 (14)
C2—C1—C6—C5	0.9 (2)	O2—N2—C13—C12	−0.2 (2)
C7—C1—C6—C5	−178.44 (14)	O3—N2—C13—C12	179.82 (14)
C2—C1—C7—C8	−171.67 (14)	O2—N2—C13—C14	179.28 (14)
C6—C1—C7—C8	7.6 (2)	O3—N2—C13—C14	−0.7 (2)
C1—C7—C8—C9	179.17 (14)	C12—C13—C14—C15	−1.0 (2)
C10—N1—C9—O1	0.5 (2)	N2—C13—C14—C15	179.59 (13)
C10—N1—C9—C8	−179.20 (14)	C13—C14—C15—C10	0.1 (2)
C7—C8—C9—O1	0.8 (2)	C11—C10—C15—C14	0.8 (2)
C7—C8—C9—N1	−179.53 (14)	N1—C10—C15—C14	179.72 (13)
C9—N1—C10—C11	−8.3 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O3^{i}	0.88	2.13	2.991 (2)	166
C5—H5···O2^{ii}	0.95	2.58	3.519 (2)	168

Symmetry codes: (i) −*x*, *y*+1/2, −*z*+3/2; (ii) *x*, *y*+1, *z*.