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N-(4-Nitrophenyl)cinnamamide

Aamer Saeed,^a Rasheed Ahmad Khera,^a Muhammad Shahid^b and Masood Parvez^{c*}^aDepartment of Chemistry, Quaid-i-Azam University, Islamabad 45320, Pakistan,^bHamdard Institute of Pharmaceutical Sciences, Hamdard University, Islamabad Campus, Pakistan, and ^cDepartment of Chemistry, The University of Calgary, 2500 University Drive NW, Calgary, Alberta, Canada T2N 1N4

Correspondence e-mail: aamersaeed@yahoo.com

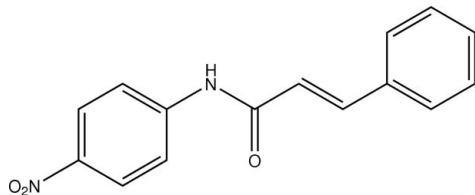
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Key indicators: single-crystal X-ray study; $T = 173$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.043; wR factor = 0.117; data-to-parameter ratio = 15.9.

In the molecule of the title compound, $\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_3$, the dihedral angle between the rings is $3.04(8)^\circ$. The central NOC_3 fragment is planar [maximum deviation = $0.005(3)$ Å] and is oriented at dihedral angles of $8.23(8)$ and $7.29(9)^\circ$ with respect to the phenyl and nitrophenyl rings, respectively. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{O}$ and $\text{C}-\text{H}\cdots\text{O}$ interactions link the molecules into a two-dimensional network. $\pi-\pi$ 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

$\text{C}_{15}\text{H}_{12}\text{N}_2\text{O}_3$
 $M_r = 268.27$
 Monoclinic, $P2_1/c$
 $a = 5.903(3)$ Å
 $b = 15.050(9)$ Å
 $c = 14.388(9)$ Å
 $\beta = 95.38(3)^\circ$

$V = 1272.6(13)$ Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 0.10$ mm⁻¹
 $T = 173$ K
 $0.20 \times 0.18 \times 0.16$ 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 $I > 2\sigma(I)$
 $R_{\text{int}} = 0.051$

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
 $\Delta\rho_{\text{max}} = 0.17$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.20$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|--|--------------|--------------------|-------------|----------------------|
| $\text{N1}-\text{H1}\cdots\text{O3}^{\text{i}}$ | 0.88 | 2.13 | 2.991(2) | 166 |
| $\text{C5}-\text{H5}\cdots\text{O2}^{\text{ii}}$ | 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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supplementary materials

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***N*-(4-Nitrophenyl)cinnamamide**

A. Saeed, R. A. Khera, M. Shahid and M. Parvez

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 NO₂ group revealed only four entries containing 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—Cg2ⁱ [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.

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 CHCl₃ 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 CHCl₃ and washed consecutively with aq 1.0 M HCl and saturated aq NaHCO₃. 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 C₁₅H₁₂N₂O₃: C, 67.16; H, 4.51; N, 10.44; found: C, 67.21; H, 4.59; N, 10.41.

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).

Figures

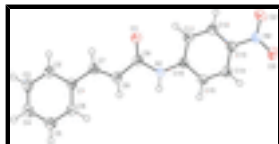


Fig. 1. The molecular structure of the title molecule with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level

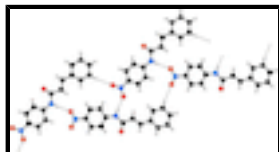


Fig. 2. A partial packing diagram. Hydrogen bonds are shown as dashed lines.

N-(4-Nitrophenyl)cinnamamide

Crystal data

$C_{15}H_{12}N_2O_3$

$M_r = 268.27$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2ybc$

$a = 5.903\ (3)\ \text{\AA}$

$b = 15.050\ (9)\ \text{\AA}$

$c = 14.388\ (9)\ \text{\AA}$

$\beta = 95.38\ (3)^\circ$

$V = 1272.6\ (13)\ \text{\AA}^3$

$Z = 4$

$F_{000} = 560$

$D_x = 1.400\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 10408 reflections

$\theta = 3.1\text{--}27.4^\circ$

$\mu = 0.10\ \text{mm}^{-1}$

$T = 173\ \text{K}$

Block, colorless

$0.20 \times 0.18 \times 0.16\ \text{mm}$

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 173\ \text{K}$

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 $I > 2\sigma(I)$

$R_{\text{int}} = 0.051$

$\theta_{\max} = 27.4^\circ$

$\theta_{\min} = 3.1^\circ$

$h = -7 \rightarrow 7$

$k = -18 \rightarrow 19$

$l = -18 \rightarrow 18$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.043$

$wR(F^2) = 0.117$

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.2254P]$

| | |
|--|--|
| $S = 1.07$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 2886 reflections | $(\Delta/\sigma)_{\max} < 0.001$ |
| 181 parameters | $\Delta\rho_{\max} = 0.17 \text{ e } \text{\AA}^{-3}$ |
| Primary atom site location: structure-invariant direct methods | $\Delta\rho_{\min} = -0.20 \text{ e } \text{\AA}^{-3}$ |
| | Extinction correction: none |

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 (\AA^2)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| 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) |

supplementary materials

| | | | | |
|-----|------------|--------------|--------------|------------|
| 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 (\AA^2)

| | 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 (\AA , $^\circ$)

| | | | |
|--------|-------------|---------|-----------|
| 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, °)

| <i>D</i> —H··· <i>A</i> | <i>D</i> —H | H··· <i>A</i> | <i>D</i> ··· <i>A</i> | <i>D</i> —H··· <i>A</i> |
|-------------------------|-------------|---------------|-----------------------|-------------------------|
| N1—H1···O3 ⁱ | 0.88 | 2.13 | 2.991 (2) | 166 |

supplementary materials

C5—H5 \cdots O2ⁱⁱ

0.95

2.58

3.519 (2)

168

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

Fig. 1

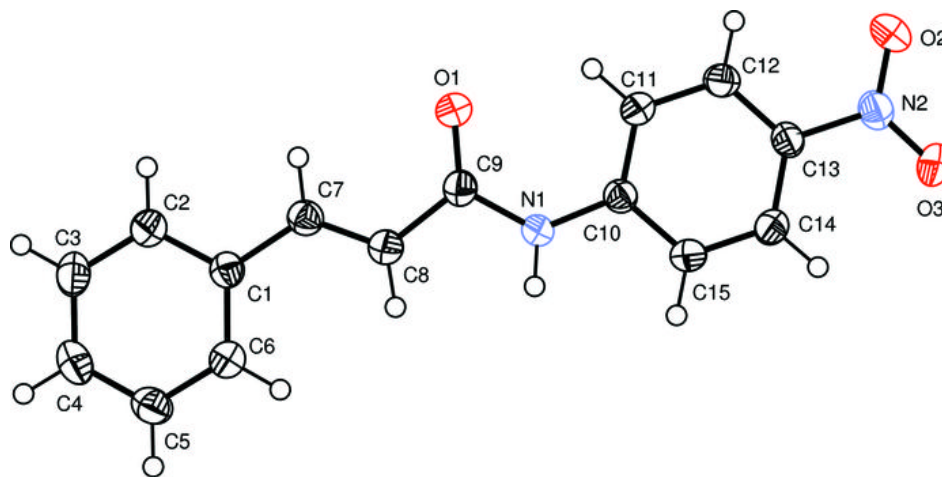


Fig. 2

