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N-(4-Nitrophenyl)-*N*′-phenylsuccinamide

Ray J. Butcher,[a] Jerry P. Jasinski,[b]* H. J. Ravindra[c] and S. M. Dharmaprakash[c]

[a]Department of Chemistry, Howard University, 525 College Street NW, Washington, DC 20059, USA, [b]Department of Chemistry, Keene State College, 229 Main Street, Keene, NH 03435-2001, USA, and [c]Department of Physics, Mangalore University, Mangalagangotri 574199, India
Correspondence e-mail: jjasinski@keene.edu

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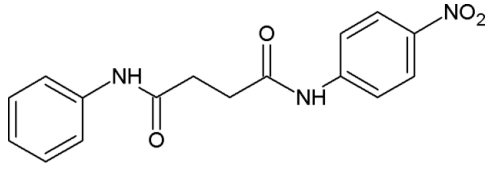
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.054; wR factor = 0.149; data-to-parameter ratio = 20.5.

In the title compound, $C_{16}H_{15}N_3O_4$, the dihedral angle between the two benzene ring is 16.66 (6)°. The molecule crystallizes in a centrosymmetric space group and hence does not exhibit nonlinear optical second harmonic generation properties. The angle between the mean plane of the 4-nitrophenyl group and the adjacent NCO group is 26.2 (8)°, while the angle between the mean plane of the phenyl ring and its adjacent NCO group is 40.8 (5)°. The dihedral angle between the two NCO groups is 5.2 (3)°. The crystal packing is stabilized by intramolecular C—H···O and intermolecular N—H···O interactions, which link the molecules into chains along the *b* axis in the *bc* plane, with the phenyl rings arranged oblique to this plane.

Related literature

For related structures, see: Crass *et al.* (1996); Anjum *et al.* (2005). For related literature, see: Ravindra *et al.* (2006); Glidewell *et al.* (2005); Munn & Ironside (1993).



Experimental

Crystal data

$C_{16}H_{15}N_3O_4$
M_r = 313.31
Triclinic, $P\overline{1}$
a = 5.7585 (4) Å
b = 9.8447 (8) Å
c = 12.9961 (10) Å
α = 79.216 (1)°
β = 79.014 (1)°
γ = 83.779 (1)°
V = 708.46 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 100 K
0.60 × 0.53 × 0.40 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan *SADABS* (Sheldrick, 2004)
T_{min} = 0.802, T_{max} = 1.000
(expected range = 0.768–0.958)
8553 measured reflections
4260 independent reflections
3904 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.054
$wR(F^2)$ = 0.149
S = 1.05
4260 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O2^{i}	0.88	2.03	2.9066 (12)	173
N2—H2B···O1^{ii}	0.88	2.10	2.9478 (12)	162
C6—H6A···O1	0.95	2.42	2.9271 (15)	113

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

Data collection: *APEX2* (Bruker, 2006); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker 2000); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2535).

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supplementary materials

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N-(4-Nitrophenyl)-*N*'-phenylsuccinamide

R. J. Butcher, J. P. Jasinski, H. J. Ravindra and S. M. Dharmaprakash

Comment

Organic nonlinear optical (NLO) materials are of increasing interest due to their large second harmonic conversion efficiency, ultra fast response, high laser damage resistance, and flexibility they offer to tune the nonlinear optical properties through structure modification [Munn & Ironside (1993)]. Due to the presence of inversion symmetry in **(I)**, the second harmonic response is zero. However, it exhibits third order nonlinear optical properties (nonlinear absorption and nonlinear refraction). The detailed measurement on the third order nonlinear properties of **(I)** has not yet performed. In order to further understand the structure-property relationship of these compounds, the title compound **(I)** has been synthesized and its crystal structure is reported.

The geometric parameters for **(I)** are normal. The C8—C9 bond length of 1.5246 (15)Å is in good agreement with the three isomeric *N*-(*p*-chlorophenyl)succinimides [Glidewell *et al.* (2005); C8—C9 = 1.5276 (19), 1.518 (3) and 1.524 (5) Å] (Fig. 1). The dihedral angle between the two benzene rings [C1—C6 and C11—C16] is 16.66 (6)°. The molecule crystallizes in a cetrosymmetric space group and hence does not exhibit second order nonlinear optical properties. The angle between the mean plane of the 4-nitrophenyl group and the adjacent N1–C7–O1 group is 26.2 (8)° while the angle between the mean plane of the benzene ring and its adjacent N2–C10–O2 group is 40.8 (5)°. The dihedral angle between the two N–C–O groups is 5.2 (3)°. The mean plane through the succinic acid fragment (C7—C10) makes the dihedral angle of 3.26 (9)° and 14.60 (9)° with the C1—C6 and C11—C16 benzene rings, respectively. Crystal packing is stabilized by intermolecular N—H—O interactions which link the molecules into chains along the *b* axis in the *bc* plane with the phenyl rings arranged oblique to this plane (Fig. 2).

Experimental

Aniline [1.395 (9) g, 0.015 mole] and *p*-nitrophenylsuccinamic acid [2.381 (1) g, 0.01 mole] were mixed in a test tube and the mixture was heated to 140° for 3 h. After cooling the solid residue was washed with dilute HCl to remove excess aniline and dried. Purification was carried out by successive recrystallization from a dimethylformamide (DMF) solution. Crystal growth was achieved by the slow evaporation of a DMF solution of **(I)**. Analysis found: C 61.29, H 4.52, N 13.38; $C_{16}H_{15}N_3O_4$ requires: C 61.33, H 4.78, N 13.41.

Refinement

The amide hydrogen atoms (H1A & H2B) were located in a difference Fourier map and along with all other H atoms were placed in their calculated positions and then refined using the riding model with N—H = 0.88Å and C—H = 0.95 to 0.99 Å, and with U_{iso}(H) = 1.17–1.22U_{eq}(C,*N*). The maximum residual electron density peaks of 0.72 and −0.32 e Å^3, were located at 0.68 from C13 and 0.50Å from N3. Owing to the poor diffraction quality of the crystal, the range of Tmax to Tmin is large (0.82).

Figures

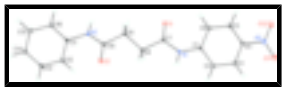

Fig. 1. Molecular structure of the title compound, showing atom labeling and 50% probability displacement ellipsoids.

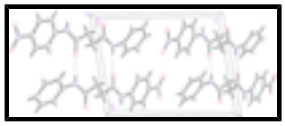

Fig. 2. Packing diagram of $C_{16}H_{15}N_3O_4$, viewed down the *a* axis. Dashed lines indicate intermolecular hydrogen bonding.

N-(4-nitrophenyl)-*N*'-phenylsuccinamide

Crystal data

$C_{16}H_{15}N_3O_4$	$Z = 2$
$M_r = 313.31$	$F_{000} = 328$
Triclinic, $P\bar{1}$	$D_x = 1.469$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 5.7585$ (4) Å	Cell parameters from 6328 reflections
$b = 9.8447$ (8) Å	$\theta = 2.4$–30.5º
$c = 12.9961$ (10) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 79.2160$ (10)º	$T = 100$ K
$\beta = 79.0140$ (10)º	Block, colorless
$\gamma = 83.7790$ (10)º	0.60 × 0.53 × 0.40 mm
$V = 708.46$ (9) Å^3	

Data collection

Bruker SMART CCD area detector diffractometer	4260 independent reflections
Radiation source: fine-focus sealed tube	3904 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.014$
$T = 100$ K	$\theta_{max} = 30.5$º
φ and ω scans	$\theta_{min} = 1.6$º
Absorption correction: multi-scan Sadabs (Sheldrick, 2004)	$h = -8 \rightarrow 8$
$T_{min} = 0.802$, $T_{max} = 1.000$	$k = -14 \rightarrow 14$
8553 measured reflections	$l = -17 \rightarrow 18$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.054$	H-atom parameters constrained
$wR(F^2) = 0.149$	$w = 1/[\sigma^2(F_o^2) + (0.0918P)^2 + 0.2598P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.05	$(\Delta/\sigma)_{max}$ = 0.003
4260 reflections	$\Delta\rho_{max}$ = 0.72 e Å^{-3}
208 parameters	$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Primary atom site location: structure-invariant direct methods	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 $F^2 > 2\text{sigma}(F^2)$ 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	0.20220 (15)	0.59779 (8)	0.11503 (7)	0.0216 (2)
O2	0.85535 (16)	0.89058 (8)	−0.09865 (8)	0.0238 (2)
O31	−0.94624 (17)	0.83821 (11)	0.42542 (8)	0.0303 (2)
O32	−0.83201 (19)	0.62538 (11)	0.48486 (9)	0.0339 (2)
N1	0.06558 (16)	0.81592 (9)	0.14504 (8)	0.01558 (19)
H1A	0.1019	0.9028	0.1300	0.019*
N2	0.97801 (16)	0.67817 (9)	−0.14277 (7)	0.01529 (19)
H2B	0.9512	0.5897	−0.1272	0.018*
N3	−0.79896 (19)	0.73754 (12)	0.42692 (9)	0.0237 (2)
C1	−0.14639 (18)	0.78803 (10)	0.21684 (8)	0.0142 (2)
C2	−0.3242 (2)	0.89650 (11)	0.21885 (9)	0.0192 (2)
H2A	−0.2980	0.9824	0.1725	0.023*
C3	−0.5377 (2)	0.87974 (13)	0.28773 (10)	0.0215 (2)
H3A	−0.6589	0.9533	0.2893	0.026*
C4	−0.5715 (2)	0.75360 (12)	0.35439 (9)	0.0184 (2)
C5	−0.3970 (2)	0.64476 (12)	0.35496 (9)	0.0193 (2)
H5A	−0.4238	0.5596	0.4021	0.023*
C6	−0.1823 (2)	0.66201 (11)	0.28562 (9)	0.0175 (2)
H6A	−0.0608	0.5886	0.2850	0.021*
C7	0.22059 (18)	0.72342 (11)	0.09634 (8)	0.0147 (2)
C8	0.41412 (19)	0.79024 (11)	0.01248 (9)	0.0165 (2)
H8A	0.4492	0.8769	0.0327	0.020*
H8B	0.3566	0.8150	−0.0562	0.020*
C9	0.64177 (19)	0.69581 (10)	−0.00172 (8)	0.0152 (2)
H9A	0.7002	0.6710	0.0668	0.018*
H9B	0.6077	0.6092	−0.0224	0.018*
C10	0.83239 (19)	0.76554 (11)	−0.08602 (8)	0.0151 (2)

C11	1.17126 (19)	0.71785 (11)	−0.22565 (8)	0.0145 (2)
C12	1.1442 (2)	0.83097 (12)	−0.30570 (9)	0.0190 (2)
H12A	0.9966	0.8846	−0.3048	0.023*
C13	1.3342 (2)	0.86508 (13)	−0.38702 (10)	0.0230 (2)
H13A	1.3166	0.9433	−0.4409	0.028*
C14	1.5494 (2)	0.78587 (13)	−0.39017 (10)	0.0236 (3)
H14A	1.6781	0.8092	−0.4463	0.028*
C15	1.5752 (2)	0.67233 (13)	−0.31067 (10)	0.0233 (2)
H15A	1.7217	0.6175	−0.3127	0.028*
C16	1.3867 (2)	0.63844 (12)	−0.22772 (9)	0.0188 (2)
H16A	1.4054	0.5615	−0.1729	0.023*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0215 (4)	0.0110 (4)	0.0287 (4)	−0.0031 (3)	0.0062 (3)	−0.0044 (3)
O2	0.0255 (4)	0.0119 (4)	0.0305 (5)	−0.0060 (3)	0.0085 (3)	−0.0058 (3)
O31	0.0197 (4)	0.0355 (5)	0.0326 (5)	0.0023 (4)	0.0018 (4)	−0.0065 (4)
O32	0.0299 (5)	0.0304 (5)	0.0359 (6)	−0.0092 (4)	0.0064 (4)	−0.0003 (4)
N1	0.0159 (4)	0.0096 (4)	0.0194 (4)	−0.0019 (3)	0.0021 (3)	−0.0026 (3)
N2	0.0158 (4)	0.0104 (4)	0.0176 (4)	−0.0025 (3)	0.0025 (3)	−0.0018 (3)
N3	0.0194 (5)	0.0279 (5)	0.0232 (5)	−0.0049 (4)	0.0006 (4)	−0.0053 (4)
C1	0.0143 (4)	0.0130 (4)	0.0153 (5)	−0.0020 (3)	−0.0005 (3)	−0.0037 (3)
C2	0.0192 (5)	0.0141 (5)	0.0215 (5)	0.0014 (4)	−0.0006 (4)	−0.0005 (4)
C3	0.0172 (5)	0.0211 (5)	0.0241 (5)	0.0038 (4)	−0.0012 (4)	−0.0042 (4)
C4	0.0156 (5)	0.0223 (5)	0.0174 (5)	−0.0036 (4)	0.0001 (4)	−0.0056 (4)
C5	0.0209 (5)	0.0176 (5)	0.0175 (5)	−0.0034 (4)	0.0014 (4)	−0.0019 (4)
C6	0.0186 (5)	0.0141 (4)	0.0176 (5)	0.0002 (4)	0.0002 (4)	−0.0014 (4)
C7	0.0142 (4)	0.0122 (4)	0.0168 (5)	−0.0019 (3)	0.0002 (3)	−0.0029 (3)
C8	0.0166 (5)	0.0118 (4)	0.0187 (5)	−0.0021 (3)	0.0023 (4)	−0.0012 (3)
C9	0.0153 (4)	0.0118 (4)	0.0165 (5)	−0.0028 (3)	0.0019 (4)	−0.0013 (3)
C10	0.0149 (4)	0.0130 (4)	0.0165 (5)	−0.0025 (3)	0.0004 (4)	−0.0029 (3)
C11	0.0143 (4)	0.0132 (4)	0.0157 (5)	−0.0029 (3)	0.0002 (3)	−0.0036 (3)
C12	0.0185 (5)	0.0174 (5)	0.0186 (5)	−0.0013 (4)	0.0000 (4)	−0.0001 (4)
C13	0.0251 (6)	0.0229 (5)	0.0182 (5)	−0.0055 (4)	0.0016 (4)	0.0003 (4)
C14	0.0193 (5)	0.0297 (6)	0.0211 (5)	−0.0073 (4)	0.0044 (4)	−0.0073 (4)
C15	0.0150 (5)	0.0280 (6)	0.0268 (6)	0.0004 (4)	−0.0003 (4)	−0.0091 (5)
C16	0.0171 (5)	0.0184 (5)	0.0201 (5)	0.0013 (4)	−0.0027 (4)	−0.0037 (4)

Geometric parameters (Å, °)

O1—C7	1.2273 (13)	C6—H6A	0.9500
O2—C10	1.2293 (13)	C7—C8	1.5133 (14)
O31—N3	1.2324 (14)	C8—C9	1.5246 (15)
O32—N3	1.2256 (15)	C8—H8A	0.9900
N1—C7	1.3605 (13)	C8—H8B	0.9900
N1—C1	1.4067 (13)	C9—C10	1.5166 (14)
N1—H1A	0.8800	C9—H9A	0.9900
N2—C10	1.3536 (13)	C9—H9B	0.9900

N2—C11	1.4252 (13)	C11—C16	1.3913 (15)
N2—H2B	0.8800	C11—C12	1.3918 (15)
N3—C4	1.4655 (15)	C12—C13	1.3901 (15)
C1—C6	1.3968 (15)	C12—H12A	0.9500
C1—C2	1.3973 (14)	C13—C14	1.3889 (18)
C2—C3	1.3820 (16)	C13—H13A	0.9500
C2—H2A	0.9500	C14—C15	1.3890 (18)
C3—C4	1.3842 (17)	C14—H14A	0.9500
C3—H3A	0.9500	C15—C16	1.3963 (16)
C4—C5	1.3873 (16)	C15—H15A	0.9500
C5—C6	1.3903 (15)	C16—H16A	0.9500
C5—H5A	0.9500		
C7—N1—C1	127.19 (9)	C9—C8—H8A	109.1
C7—N1—H1A	116.4	C7—C8—H8B	109.1
C1—N1—H1A	116.4	C9—C8—H8B	109.1
C10—N2—C11	125.28 (9)	H8A—C8—H8B	107.8
C10—N2—H2B	117.4	C10—C9—C8	111.42 (9)
C11—N2—H2B	117.4	C10—C9—H9A	109.3
O32—N3—O31	123.96 (11)	C8—C9—H9A	109.3
O32—N3—C4	118.41 (10)	C10—C9—H9B	109.3
O31—N3—C4	117.63 (10)	C8—C9—H9B	109.3
C6—C1—C2	120.11 (10)	H9A—C9—H9B	108.0
C6—C1—N1	123.70 (9)	O2—C10—N2	123.39 (10)
C2—C1—N1	116.17 (9)	O2—C10—C9	122.10 (9)
C3—C2—C1	120.47 (10)	N2—C10—C9	114.47 (9)
C3—C2—H2A	119.8	C16—C11—C12	120.11 (10)
C1—C2—H2A	119.8	C16—C11—N2	118.88 (10)
C2—C3—C4	118.67 (10)	C12—C11—N2	120.97 (10)
C2—C3—H3A	120.7	C13—C12—C11	119.69 (11)
C4—C3—H3A	120.7	C13—C12—H12A	120.2
C3—C4—C5	122.05 (10)	C11—C12—H12A	120.2
C3—C4—N3	117.98 (10)	C14—C13—C12	120.62 (11)
C5—C4—N3	119.97 (10)	C14—C13—H13A	119.7
C4—C5—C6	119.13 (10)	C12—C13—H13A	119.7
C4—C5—H5A	120.4	C15—C14—C13	119.55 (11)
C6—C5—H5A	120.4	C15—C14—H14A	120.2
C5—C6—C1	119.56 (10)	C13—C14—H14A	120.2
C5—C6—H6A	120.2	C14—C15—C16	120.30 (11)
C1—C6—H6A	120.2	C14—C15—H15A	119.9
O1—C7—N1	123.76 (10)	C16—C15—H15A	119.9
O1—C7—C8	122.49 (9)	C11—C16—C15	119.73 (11)
N1—C7—C8	113.69 (9)	C11—C16—H16A	120.1
C7—C8—C9	112.61 (9)	C15—C16—H16A	120.1
C7—C8—H8A	109.1		
C7—N1—C1—C6	30.18 (17)	O1—C7—C8—C9	−30.73 (15)
C7—N1—C1—C2	−151.52 (11)	N1—C7—C8—C9	151.83 (10)
C6—C1—C2—C3	−0.80 (17)	C7—C8—C9—C10	−179.91 (9)
N1—C1—C2—C3	−179.16 (10)	C11—N2—C10—O2	−1.76 (18)

C1—C2—C3—C4	−0.03 (18)	C11—N2—C10—C9	−179.55 (10)
C2—C3—C4—C5	0.83 (18)	C8—C9—C10—O2	35.54 (15)
C2—C3—C4—N3	−179.99 (10)	C8—C9—C10—N2	−146.63 (10)
O32—N3—C4—C3	178.70 (12)	C10—N2—C11—C16	135.14 (12)
O31—N3—C4—C3	−0.99 (17)	C10—N2—C11—C12	−47.19 (16)
O32—N3—C4—C5	−2.09 (17)	C16—C11—C12—C13	−0.71 (17)
O31—N3—C4—C5	178.21 (11)	N2—C11—C12—C13	−178.36 (10)
C3—C4—C5—C6	−0.79 (18)	C11—C12—C13—C14	1.16 (18)
N3—C4—C5—C6	−179.96 (10)	C12—C13—C14—C15	−0.60 (19)
C4—C5—C6—C1	−0.06 (17)	C13—C14—C15—C16	−0.41 (19)
C2—C1—C6—C5	0.83 (17)	C12—C11—C16—C15	−0.28 (17)
N1—C1—C6—C5	179.07 (10)	N2—C11—C16—C15	177.41 (10)
C1—N1—C7—O1	−5.20 (18)	C14—C15—C16—C11	0.85 (18)
C1—N1—C7—C8	172.20 (10)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1A···O2^{i}	0.88	2.03	2.9066 (12)	173
N2—H2B···O1^{ii}	0.88	2.10	2.9478 (12)	162
C6—H6A···O1	0.95	2.42	2.9271 (15)	113

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

Fig. 1

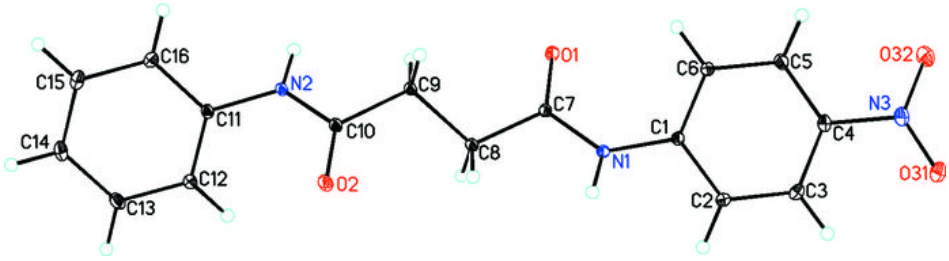
C16
C15
N2
C11
C10
C9
O1
C7
C6
C5
O32
C14
C12
O2
C8
N1
C1
C4
N3
C13
C2
C3
O31

Fig. 2