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N-(2-Nitrophenyl)benzamide

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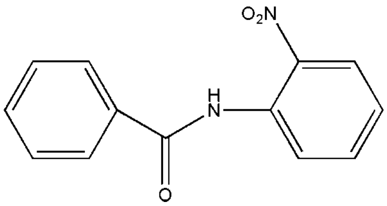
Key indicators: single-crystal X-ray study; *T* = 89 K; mean σ(C–C) = 0.001 Å; *R* factor = 0.041; *wR* factor = 0.118; data-to-parameter ratio = 23.6.

In the title compound, $C_{13}H_{10}N_2O_3$, the central C–C(=O)–N–C amide unit makes dihedral angles of 21.68 (4) and 19.08 (4)°, respectively, with the phenyl and nitrobenzene rings. The two aromatic rings are inclined at 3.74 (3)° and the nitro group is skewed out of the attached benzene ring plane by 18.55 (8)°. An intramolecular N—H···O interaction to an O atom of the nitro substituent generates an *S*(6) ring motif. In the crystal, C—H···O contacts generate two centrosymmetric ring systems with $R_2^2(14)$ and $R_2^2(20)$ graph-set motifs, forming zigzag chains down the *a* axis. π–π interactions between adjacent phenyl and nitrobenzene rings [centroid–centroid distance = 3.6849 (6) Å] also form centrosymmetric dimers. These and an additional C—H···O hydrogen bond generate an extensive three-dimensional network structure.

Related literature

For the biological activity of benzamide derivatives see Saeed *et al.* (2008). For related structures, see: Cronin *et al.* (2000); Glidewell *et al.* (2004); Wardell *et al.* (2005). For reference structural data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{13}H_{10}N_2O_3$
$M_r = 242.23$
Monoclinic, $P2_1/n$
$a = 7.2061 (5)$ Å
$b = 7.4253 (5)$ Å
$c = 20.6031 (13)$ Å
$\beta = 93.560 (4)°$
$V = 1100.29 (13)$ Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 0.11$ mm^{-1}
$T = 89$ K
0.24 × 0.17 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2006)
$T_{min} = 0.852$, $T_{max} = 0.991$
20195 measured reflections
3948 independent reflections
3098 reflections with $I > 2\sigma(I)$
$R_{int} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
$wR(F^2) = 0.118$
$S = 1.06$
3948 reflections
167 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max} = 0.49$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O3	0.887 (16)	1.927 (15)	2.6361 (11)	135.7 (13)
C10—H10···O2^{i}	0.95	2.57	3.2254 (12)	126
C6—H6···O3^{ii}	0.95	2.65	3.5122 (12)	151
C12—H12···O1^{iii}	0.95	2.48	3.3695 (12)	157

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

Data collection: *APEX2* (Bruker 2006); cell refinement: *APEX2* and *SAINT* (Bruker 2006); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008) and *TITAN2000* (Hunter & Simpson, 1999); molecular graphics: *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*, *enCIFer* (Allen *et al.*, 2004), *PLATON* (Spek, 2009) and *publCIF* (Westrip, 2009).

We thank the University of Otago for purchase of the diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2824).

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supplementary materials

Acta Cryst. (2009). E**65**, o1845 [**doi:10.1107/S1600536809024271**]

N-(2-Nitrophenyl)benzamide

A. Saeed and **J. Simpson**

Comment

The biological activity and applications of benzamide derivatives have been described in an earlier paper (Saeed *et al.* 2008*a*). This paper reports the structure of a nitrophenyl benzamide derivative, (I), Fig. 1. The C2–C1(O1)–N1–C8 amide unit makes dihedral angles of 21.68 (4) ° and 19.08 (4) ° with the C2–C7 and C8–C13 rings respectively. The two aromatic rings are inclined at 3.74 (3)° with the nitro group skewed out of the C8–C13 ring plane by 18.55 (8)°. An intramolecular N1—H1N···O3 interaction generates an S6 ring motif. Bond lengths in the molecule are normal (Allen *et al.* 1987) and comparable to those observed in similar structures (Cronin *et al.*, 2000; Glidewell *et al.*, 2004; Wardell *et al.*, 2005).

In the crystal C12—H12···O1 and C6—H6···O3 contacts generate two centrosymmetric ring systems with $R_2^2(14)$ and $R_2^2(20)$ graph set motifs respectively, forming zigzag chains down the *a* axis, Fig 2. π–π interactions between adjacent C2–C7 and C8–C13 rings [*Cg*···*Cg* distance 3.6849 (6) Å] also form centrosymmetric dimers, Fig 3. These and an additional C10—H10···O2 hydrogen bond generate an extensive three dimensional network structure, Fig. 4.

Experimental

Freshly distilled benzoyl chloride (5.4 mmol) in $CHCl_3$ was treated with 2-nitroaniline (21.6 mmol) under a nitrogen atmosphere at reflux for 3 h. Upon cooling, the reaction mixture was diluted with $CHCl_3$ and washed consecutively with aq 1 *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 $CHCl_3$ afforded the title compound (81%) as white plates: Analysis calculated for $C_{13}H_{10}N_2O_3$: C 64.46, H 4.16, N 11.56%; found: C 64.39, H 4.21, N 11.71%

Refinement

The H atom bound to N1 was located in a difference Fourier map and refined freely with an isotropic displacement parameter. The remaining aromatic H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.95 Å, $U_{iso}=1.2U_{eq}$ (C).

Figures

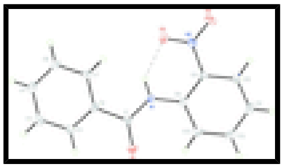

Fig. 1. The structure of (I) with displacement ellipsoids for the non-hydrogen atoms drawn at the 50% probability level. An intramolecular hydrogen bond is drawn as a dashed line.

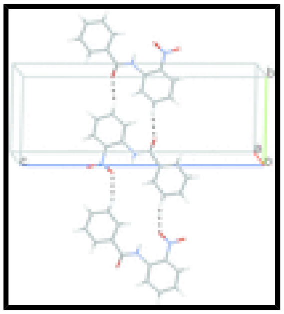

Fig. 2. Pairs of centrosymmetric dimers forming a chain running down *b* axis. Hydrogen bonds are drawn as dashed lines.

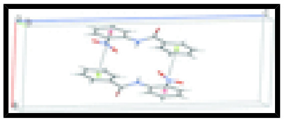

Fig. 3. Centrosymmetric dimers formed through π–π stacking interactions shown as dotted lines with coloured circles representing the ring centroids. The symmetry operation relating the two molecules is 1 - *x*, -*y*, 1 - *z*.

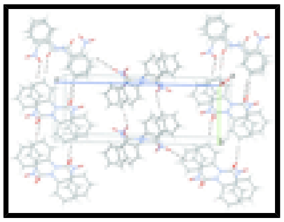

Fig. 4. Crystal packing of (I) viewed down the *a* axis.

N-(2-Nitrophenyl)benzamide

Crystal data

$C_{13}H_{10}N_2O_3$

$M_r = 242.23$

Monoclinic, $P2_1/n$

Hall symbol: -P 2yn

$a = 7.2061$ (5) Å

$b = 7.4253$ (5) Å

$c = 20.6031$ (13) Å

β = 93.560 (4)°

$V = 1100.29$ (13) Å^3

$Z = 4$

$F_{000} = 504$

$D_x = 1.462$ Mg m^{-3}

Mo *K*α radiation, λ = 0.71073 Å

Cell parameters from 4696 reflections

θ = 2.8–31.8°

μ = 0.11 mm^{-1}

$T = 89$ K

Plate, colourless

0.24 × 0.17 × 0.09 mm

Data collection

Bruker APEXII CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 89$ K

ω scans

Absorption correction: multi-scan (SADABS; Bruker, 2006)

$T_{min} = 0.852$, $T_{max} = 0.991$

20195 measured reflections

3948 independent reflections

3098 reflections with $I > 2\sigma(I)$

$R_{int} = 0.037$

$\theta_{max} = 33.3°$

$\theta_{min} = 3.1°$

$h = -10\rightarrow10$

$k = -11\rightarrow10$

$l = -30\rightarrow30$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.041$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.118$	$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.2001P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
3948 reflections	$\Delta\rho_{max} = 0.49$ e Å^{-3}
167 parameters	$\Delta\rho_{min} = -0.27$ 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 $F^2 > \sigma(F^2)$ 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}
N1	0.73812 (11)	0.03317 (11)	0.50049 (4)	0.01315 (16)
H1N	0.678 (2)	−0.064 (2)	0.5129 (7)	0.031 (4)*
O1	0.87401 (11)	0.16410 (10)	0.41448 (4)	0.01879 (17)
C1	0.78498 (13)	0.04075 (12)	0.43690 (4)	0.01259 (17)
C2	0.71690 (13)	−0.11570 (12)	0.39614 (4)	0.01239 (17)
C3	0.70064 (14)	−0.09052 (13)	0.32883 (5)	0.01564 (19)
H3	0.7315	0.0226	0.3109	0.019*
C4	0.63950 (14)	−0.23021 (14)	0.28797 (5)	0.01771 (19)
H4	0.6275	−0.2120	0.2423	0.021*
C5	0.59588 (14)	−0.39666 (14)	0.31405 (5)	0.0176 (2)
H5	0.5543	−0.4921	0.2861	0.021*
C6	0.61305 (14)	−0.42356 (13)	0.38095 (5)	0.01679 (19)
H6	0.5840	−0.5376	0.3986	0.020*
C7	0.67274 (13)	−0.28349 (13)	0.42198 (5)	0.01451 (18)
H7	0.6836	−0.3018	0.4677	0.017*
C8	0.78625 (12)	0.15306 (12)	0.55126 (4)	0.01171 (17)
C9	0.78085 (13)	0.09917 (12)	0.61677 (4)	0.01252 (17)

N2	0.72463 (12)	−0.08197 (11)	0.63520 (4)	0.01487 (17)
O2	0.76511 (13)	−0.13362 (11)	0.69076 (4)	0.0268 (2)
O3	0.63473 (11)	−0.17725 (10)	0.59477 (3)	0.01818 (16)
C10	0.82755 (13)	0.21653 (14)	0.66792 (5)	0.01574 (19)
H10	0.8235	0.1765	0.7116	0.019*
C11	0.87973 (14)	0.39107 (14)	0.65503 (5)	0.0184 (2)
H11	0.9112	0.4720	0.6897	0.022*
C12	0.88585 (14)	0.44738 (13)	0.59089 (5)	0.01733 (19)
H12	0.9218	0.5675	0.5820	0.021*
C13	0.84023 (13)	0.33090 (12)	0.53965 (5)	0.01466 (18)
H13	0.8457	0.3723	0.4962	0.018*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0166 (4)	0.0113 (4)	0.0116 (3)	−0.0039 (3)	0.0014 (3)	−0.0001 (3)
O1	0.0249 (4)	0.0136 (3)	0.0186 (3)	−0.0056 (3)	0.0078 (3)	−0.0007 (3)
C1	0.0126 (4)	0.0114 (4)	0.0139 (4)	0.0010 (3)	0.0017 (3)	0.0002 (3)
C2	0.0119 (4)	0.0119 (4)	0.0133 (4)	0.0005 (3)	0.0010 (3)	−0.0004 (3)
C3	0.0179 (4)	0.0153 (4)	0.0140 (4)	0.0009 (3)	0.0023 (3)	0.0007 (3)
C4	0.0190 (5)	0.0201 (5)	0.0139 (4)	0.0021 (4)	0.0000 (3)	−0.0023 (3)
C5	0.0149 (4)	0.0179 (5)	0.0198 (4)	0.0004 (3)	−0.0011 (3)	−0.0060 (4)
C6	0.0162 (4)	0.0127 (4)	0.0214 (5)	−0.0012 (3)	0.0006 (3)	−0.0013 (3)
C7	0.0154 (4)	0.0128 (4)	0.0153 (4)	−0.0001 (3)	0.0010 (3)	0.0005 (3)
C8	0.0102 (4)	0.0115 (4)	0.0135 (4)	0.0003 (3)	0.0009 (3)	−0.0008 (3)
C9	0.0126 (4)	0.0109 (4)	0.0140 (4)	0.0005 (3)	0.0009 (3)	−0.0002 (3)
N2	0.0181 (4)	0.0137 (4)	0.0130 (3)	0.0016 (3)	0.0023 (3)	0.0012 (3)
O2	0.0434 (5)	0.0226 (4)	0.0139 (3)	0.0000 (3)	−0.0016 (3)	0.0063 (3)
O3	0.0239 (4)	0.0138 (3)	0.0168 (3)	−0.0041 (3)	0.0013 (3)	0.0000 (2)
C10	0.0149 (4)	0.0179 (4)	0.0143 (4)	0.0022 (3)	−0.0001 (3)	−0.0030 (3)
C11	0.0158 (4)	0.0182 (5)	0.0212 (5)	−0.0008 (4)	0.0016 (4)	−0.0082 (4)
C12	0.0148 (4)	0.0125 (4)	0.0252 (5)	−0.0023 (3)	0.0054 (4)	−0.0038 (4)
C13	0.0145 (4)	0.0117 (4)	0.0180 (4)	−0.0009 (3)	0.0035 (3)	0.0000 (3)

Geometric parameters (Å, °)

N1—C1	1.3742 (11)	C7—H7	0.9500
N1—C8	1.4006 (12)	C8—C13	1.4014 (13)
N1—H1N	0.887 (16)	C8—C9	1.4107 (13)
O1—C1	1.2250 (11)	C9—C10	1.3925 (13)
C1—C2	1.4981 (13)	C9—N2	1.4617 (12)
C2—C3	1.3971 (12)	N2—O2	1.2251 (10)
C2—C7	1.3992 (13)	N2—O3	1.2439 (11)
C3—C4	1.3902 (14)	C10—C11	1.3799 (14)
C3—H3	0.9500	C10—H10	0.9500
C4—C5	1.3915 (15)	C11—C12	1.3893 (15)
C4—H4	0.9500	C11—H11	0.9500
C5—C6	1.3906 (14)	C12—C13	1.3883 (13)
C5—H5	0.9500	C12—H12	0.9500

C6—C7	1.3914 (13)	C13—H13	0.9500
C6—H6	0.9500		
C1—N1—C8	128.45 (8)	C2—C7—H7	119.9
C1—N1—H1N	117.4 (10)	N1—C8—C13	122.01 (8)
C8—N1—H1N	113.9 (10)	N1—C8—C9	120.93 (8)
O1—C1—N1	123.75 (9)	C13—C8—C9	117.06 (8)
O1—C1—C2	121.96 (8)	C10—C9—C8	121.79 (9)
N1—C1—C2	114.29 (8)	C10—C9—N2	115.92 (8)
C3—C2—C7	119.32 (9)	C8—C9—N2	122.29 (8)
C3—C2—C1	117.20 (8)	O2—N2—O3	122.11 (9)
C7—C2—C1	123.47 (8)	O2—N2—C9	118.49 (8)
C4—C3—C2	120.34 (9)	O3—N2—C9	119.38 (8)
C4—C3—H3	119.8	C11—C10—C9	119.87 (9)
C2—C3—H3	119.8	C11—C10—H10	120.1
C3—C4—C5	119.97 (9)	C9—C10—H10	120.1
C3—C4—H4	120.0	C10—C11—C12	119.39 (9)
C5—C4—H4	120.0	C10—C11—H11	120.3
C6—C5—C4	120.13 (9)	C12—C11—H11	120.3
C6—C5—H5	119.9	C13—C12—C11	121.05 (9)
C4—C5—H5	119.9	C13—C12—H12	119.5
C5—C6—C7	119.99 (9)	C11—C12—H12	119.5
C5—C6—H6	120.0	C12—C13—C8	120.83 (9)
C7—C6—H6	120.0	C12—C13—H13	119.6
C6—C7—C2	120.23 (9)	C8—C13—H13	119.6
C6—C7—H7	119.9		

Hydrogen-bond geometry (Å, °)

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

Fig. 1

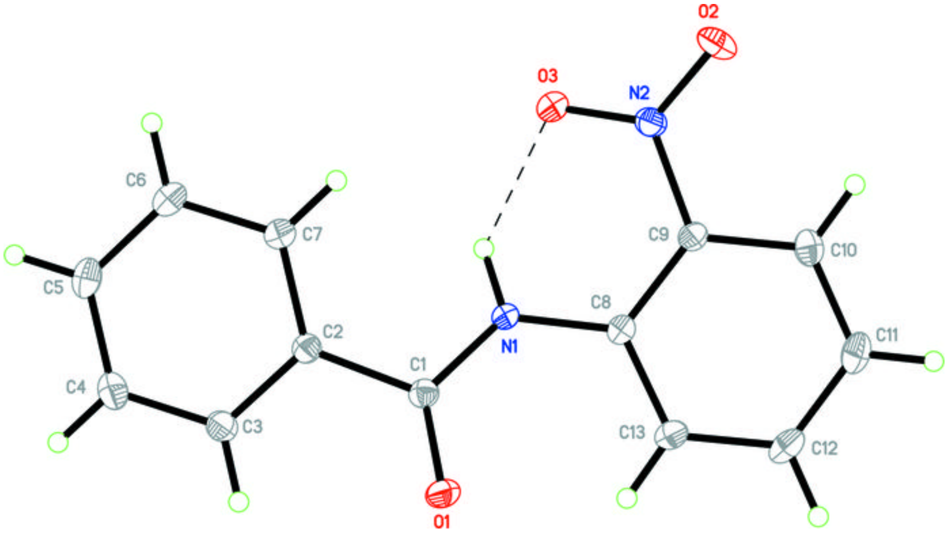

Fig. 2

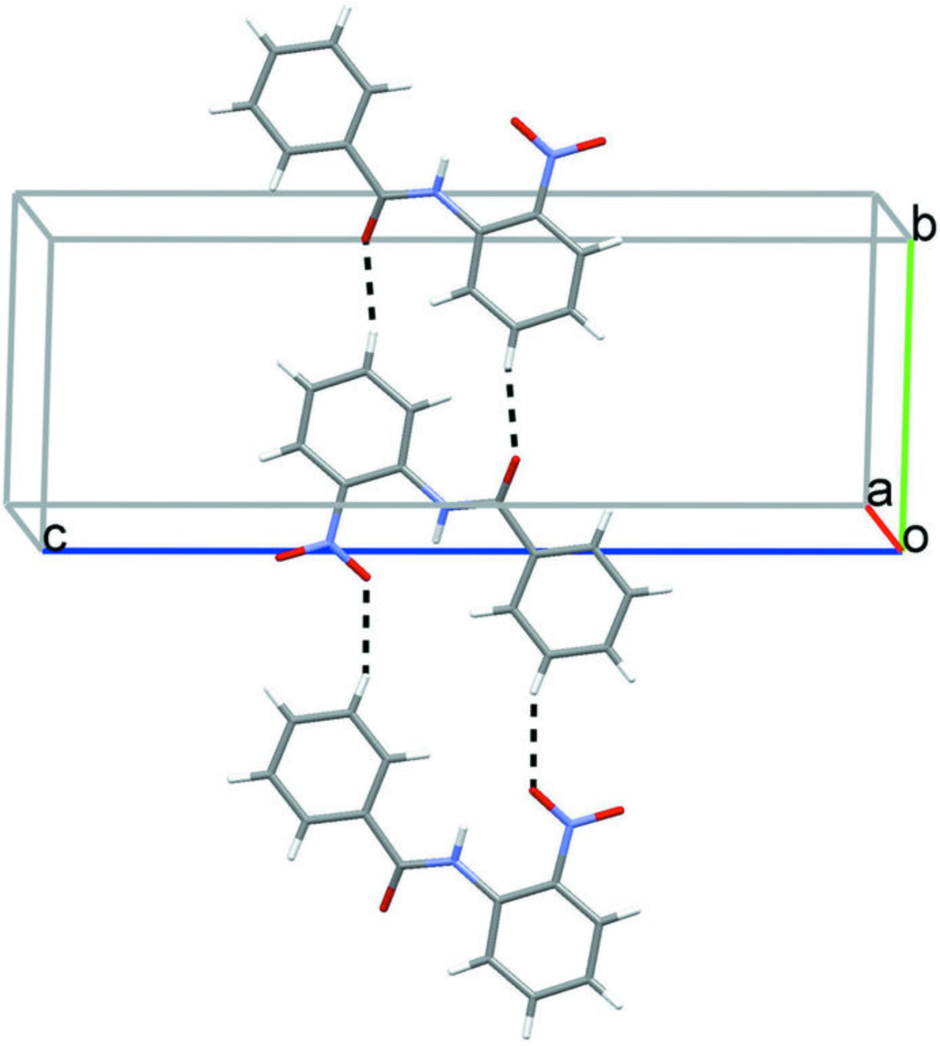

Fig. 3

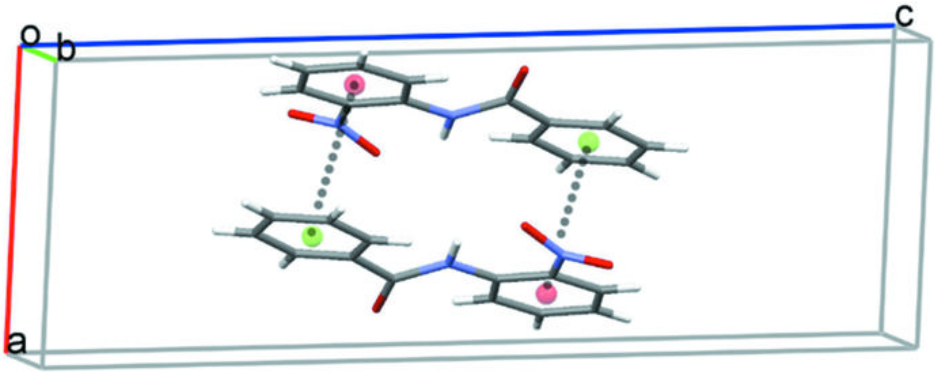

Fig. 4